

REMARKS

A Notice of Allowance has been mailed from the USPTO for the above-referenced application. The Examiner contacted the undersigned by telephone indicating that Tables 5 and 6 were not sufficiently clear for printing the forthcoming Letters Patent. Applicants submit herewith Replacement Sheets containing Tables 5 and 6. No issue of new matter arises from this submission since the Replacement Sheets are merely clearer copies of the Tables 5 and 6 as filed.

Fees

No fees are believed to be necessary in connection with this Amendment. However, if this is in error, authorization is hereby given to charge Deposit Account No. 11-1153 for any underpayment, or credit any overages.

Conclusion

If a discussion might be of assistance in resolving any issues, the Examiner is invited to telephone the undersigned.

Respectfully submitted,



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Registration No. 39,839

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Table 5

| Atomic Structure Coordinates of the Free Form of the P/CAP Bromodomain | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
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| REMARK FILENAME= /blobz/chris/BRNO_XPLOR_AHN3/structures/it/bnd_187.pdb* | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
| REMARK initial random number seed: 1,3427168211 | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
| REMARK overall bonds, angles, improper dihedrals, and torsions | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
| REMARK energies: 157.923, 9.30565, 73.153, 0, 22.1819, 36.4277, 0, 228.429 | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
| REMARK rms-dev.: 2.161568-01, 0.36411, 50.311, 1, 43.8985E-02, 0, 265303 | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
| REMARK note, cdih | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
| REMARK violations: 2, 0 | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
| REMARK DATE:20-Nov-98 06:51:33 | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
| REMARK created by user: | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
| ATOM 1 CA GLY 1 27.208 16.825 -6.349 1.00 0.00 | ATOM 432 N IYS 6 22.756 3.805 -5.800 1.00 0.00 | ATOM 67 N IYS 6 22.756 3.805 -5.800 1.00 0.00 | ATOM 161 HGL PRO 11 15.582 -6.715 -3.188 1.00 0.00 | ATOM 162 HGL PRO 11 15.582 -6.715 -3.188 1.00 0.00 | ATOM 163 CD PRO 11 14.324 -5.681 -3.666 1.00 0.00 | ATOM 164 HDI PRO 11 15.981 -4.682 -2.666 1.00 0.00 | ATOM 165 C PRO 11 16.195 -4.133 -3.582 1.00 0.00 | ATOM 166 S PRO 11 16.911 -5.086 -2.237 1.00 0.00 | ATOM 167 O PRO 11 13.991 -5.466 1.375 1.00 0.00 | ATOM 168 N ASP 12 15.926 4.397 0.912 1.00 0.00 | ATOM 169 RHN ASP 12 16.430 -4.508 2.276 1.00 0.00 | ATOM 170 RAH ASP 12 16.402 -5.521 2.584 1.00 0.00 | ATOM 171 RAH ASP 12 16.402 -5.521 2.584 1.00 0.00 | ATOM 172 HBL ASP 12 15.785 -2.412 3.242 1.00 0.00 | ATOM 173 HBL ASP 12 16.166 -3.873 3.399 1.00 0.00 | ATOM 174 HBL ASP 12 16.798 -3.061 1.899 1.00 0.00 | ATOM 175 CG ASP 12 18.896 -4.975 1.771 1.00 0.00 | ATOM 176 CGL ASP 12 18.870 -6.197 2.125 1.00 0.00 | ATOM 177 ODP ASP 12 19.615 -4.549 3.921 1.00 0.00 | ATOM 178 O ASP 12 19.555 -3.719 3.243 1.00 0.00 | ATOM 179 O ASP 12 14.679 -4.202 3.913 1.00 0.00 | ATOM 180 N GLN 13 15.785 -2.412 3.309 1.00 0.00 | ATOM 181 RN GLN 13 15.026 -1.546 4.181 1.00 0.00 | ATOM 182 RN GLN 13 15.155 -1.923 5.187 1.00 0.00 | ATOM 183 RN GLN 13 15.550 -0.115 6.134 1.00 0.00 | ATOM 184 RN GLN 13 15.059 -0.411 3.931 1.00 0.00 | ATOM 185 HGL GLN 13 16.510 -0.149 3.931 1.00 0.00 | ATOM 186 HGL GLN 13 15.116 -0.659 5.420 1.00 0.00 | ATOM 187 CO GLN 13 15.555 -0.255 6.226 1.00 0.00 | ATOM 188 CO GLN 13 15.289 -0.255 6.226 1.00 0.00 | ATOM 189 HGL GLN 13 15.289 -0.255 6.226 1.00 0.00 | ATOM 190 O GLN 13 14.450 -1.025 6.622 1.00 0.00 | ATOM 191 O GLN 13 14.875 -2.188 6.790 1.00 0.00 | ATOM 192 NEZ GLN 13 15.930 -2.328 7.25 1.00 0.00 | ATOM 193 HGL GLN 13 17.651 -2.328 7.25 1.00 0.00 | ATOM 194 C GLN 13 16.543 -1.085 7.507 1.00 0.00 | ATOM 195 C GLN 13 15.358 -1.566 7.507 1.00 0.00 | ATOM 196 C GLN 13 15.228 -0.566 7.507 1.00 0.00 | ATOM 197 C GLN 13 15.228 -0.566 7.507 1.00 0.00 | ATOM 198 HN GLU 14 16.176 -1.628 4.499 1.00 0.00 | ATOM 199 HN GLU 14 16.875 -2.123 5.091 1.00 0.00 | ATOM 200 HN GLU 14 17.194 -2.778 5.778 1.00 0.00 | ATOM 201 CB GLN 13 16.930 -2.123 5.778 1.00 0.00 | ATOM 202 HBL PRO 8 17.200 -1.002 9.523 1.00 0.00 | ATOM 203 HBL PRO 8 16.011 -0.245 9.523 1.00 0.00 | ATOM 204 CG LEU 14 16.796 -0.357 9.58 1.00 0.00 | ATOM 205 CG LEU 14 16.677 -0.357 9.58 1.00 0.00 | ATOM 206 CDI LEU 14 16.100 -1.352 -7.702 1.00 0.00 | ATOM 207 HDI LEU 14 16.000 -1.352 -7.702 1.00 0.00 | ATOM 208 HDI LEU 14 16.429 -0.419 -8.727 1.00 0.00 | ATOM 209 HDI LEU 14 16.760 -0.419 -8.727 1.00 0.00 | ATOM 210 HDI LEU 14 17.200 -1.002 9.523 1.00 0.00 | ATOM 211 HDI LEU 14 16.000 -0.245 9.523 1.00 0.00 | ATOM 212 HDI LEU 14 16.796 -0.357 9.58 1.00 0.00 | ATOM 213 HDI LEU 14 16.677 -0.357 9.58 1.00 0.00 | ATOM 214 CG LEU 14 16.100 -1.352 -7.702 1.00 0.00 | ATOM 215 CG LEU 14 16.052 -0.245 -7.733 1.00 0.00 | ATOM 216 CG LEU 14 16.500 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REPLACEMENT SHEET

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|------|-----|---------|----|--------|---------|--------|------|------|------|-----|---------|----|--------|--------|---------|------|------|
| ATOM | 245 | HG1 THR | 17 | 10.098 | 1.223 | 6.144 | 1.00 | 0.00 | ATOM | 349 | HG2 LBN | 22 | 0.803 | 4.94 | 3.088 | 1.00 | 0.00 |
| ATOM | 256 | HCG THR | 17 | 10.991 | 0.832 | 4.783 | 1.00 | 0.00 | ATOM | 444 | N HIS | 28 | -4.264 | 1.759 | -12.558 | 1.00 | 0.00 |
| ATOM | 257 | HCG THR | 17 | 10.078 | 0.224 | 4.720 | 1.00 | 0.00 | ATOM | 444 | O HIS | 28 | -4.083 | 1.459 | 13.454 | 1.00 | 0.00 |
| ATOM | 258 | HCG THR | 17 | 0.088 | 1.395 | 3.867 | 1.00 | 0.00 | ATOM | 445 | COD HIS | 28 | -4.569 | 1.777 | 10.377 | 1.00 | 0.00 |
| ATOM | 259 | HCG THR | 17 | 0.883 | 1.513 | 5.612 | 1.00 | 0.00 | ATOM | 446 | HOD HIS | 28 | -4.665 | 5.487 | 9.340 | 1.00 | 0.00 |
| ATOM | 260 | O THR | 17 | 1.682 | 4.886 | 5.821 | 1.00 | 0.00 | ATOM | 447 | CEI HIS | 28 | -4.567 | 3.882 | 12.859 | 1.00 | 0.00 |
| ATOM | 261 | O THR | 17 | 1.676 | 6.646 | 6.646 | 1.00 | 0.00 | ATOM | 449 | NEZ HIS | 28 | -4.719 | 3.042 | 10.886 | 1.00 | 0.00 |
| ATOM | 262 | O THR | 17 | 1.574 | 2.599 | 4.697 | 1.00 | 0.00 | ATOM | 450 | HEZ HIS | 28 | -4.915 | 3.844 | 10.367 | 1.00 | 0.00 |
| ATOM | 263 | HG1 LBN | 18 | 0.539 | 2.518 | 4.093 | 1.00 | 0.00 | ATOM | 451 | M HIS | 28 | -6.246 | -1.009 | 12.480 | 1.00 | 0.00 |
| ATOM | 264 | HG1 LBN | 18 | 0.689 | -3.302 | 4.330 | 1.00 | 0.00 | ATOM | 452 | O HIS | 28 | -6.982 | -5.568 | 8.224 | 1.00 | 0.00 |
| ATOM | 265 | HG1 LBN | 18 | 0.595 | 2.289 | 4.289 | 1.00 | 0.00 | ATOM | 453 | N HIS | 28 | -6.600 | -0.037 | 13.241 | 1.00 | 0.00 |
| ATOM | 266 | CIS LBN | 18 | 0.500 | -1.918 | 4.98 | 1.00 | 0.00 | ATOM | 454 | RN HIS | 28 | -6.048 | 0.472 | 13.779 | 1.00 | 0.00 |
| ATOM | 267 | HBL LBN | 18 | 1.700 | 4.954 | 3.965 | 1.00 | 0.00 | ATOM | 455 | CA HIS | 28 | -8.109 | 0.272 | 13.334 | 1.00 | 0.00 |
| ATOM | 268 | HBL LBN | 18 | 1.026 | 4.000 | 4.000 | 1.00 | 0.00 | ATOM | 456 | HA HIS | 28 | -8.640 | -0.668 | 13.358 | 1.00 | 0.00 |
| ATOM | 269 | CIS LBN | 18 | 0.584 | -2.849 | 2.014 | 1.00 | 0.00 | ATOM | 457 | CB HIS | 28 | -8.371 | 1.007 | 14.688 | 1.00 | 0.00 |
| ATOM | 270 | HBL LBN | 18 | 0.654 | -2.603 | 2.075 | 1.00 | 0.00 | ATOM | 458 | HE2 HIS | 28 | -9.433 | 1.018 | 14.822 | 1.00 | 0.00 |
| ATOM | 271 | CIS LBN | 18 | 0.554 | 5.503 | 1.000 | 1.00 | 0.00 | ATOM | 459 | HE2 GLN | 29 | -8.012 | 2.021 | 14.522 | 1.00 | 0.00 |
| ATOM | 272 | HBL LBN | 18 | 0.654 | -2.603 | 2.075 | 1.00 | 0.00 | ATOM | 460 | CG GLN | 29 | -7.670 | -0.275 | 11.889 | 1.00 | 0.00 |
| ATOM | 273 | HBL LBN | 18 | 0.640 | -4.442 | 0.524 | 1.00 | 0.00 | ATOM | 461 | HG1 GLN | 29 | -7.180 | -0.500 | 15.445 | 1.00 | 0.00 |
| ATOM | 274 | HBL LBN | 18 | 0.648 | -1.722 | 1.899 | 1.00 | 0.00 | ATOM | 462 | HG2 GLN | 29 | -6.929 | -1.021 | 16.203 | 1.00 | 0.00 |
| ATOM | 275 | HBL LBN | 18 | 0.518 | -0.963 | 6.365 | 1.00 | 0.00 | ATOM | 463 | CD GLN | 29 | -8.622 | -0.000 | 6.953 | 1.00 | 0.00 |
| ATOM | 276 | HBL LBN | 18 | 0.511 | -1.423 | 0.889 | 1.00 | 0.00 | ATOM | 464 | ND1 GLN | 29 | -8.354 | -0.224 | 18.047 | 1.00 | 0.00 |
| ATOM | 277 | HBL LBN | 18 | 0.549 | -2.403 | 0.000 | 1.00 | 0.00 | ATOM | 465 | NE2 GLN | 29 | -9.770 | -0.676 | 16.586 | 1.00 | 0.00 |
| ATOM | 278 | HBL LBN | 18 | 0.569 | -2.603 | 2.075 | 1.00 | 0.00 | ATOM | 466 | HE2 GLN | 29 | -9.811 | 1.000 | 0.000 | 0.00 | 0.00 |
| ATOM | 279 | C LBN | 18 | 0.637 | -4.376 | 5.349 | 1.00 | 0.00 | ATOM | 467 | CG LBN | 29 | -8.013 | -0.995 | 12.267 | 1.00 | 0.00 |
| ATOM | 280 | O LBN | 18 | 0.654 | -3.603 | 5.503 | 1.00 | 0.00 | ATOM | 468 | CH LBN | 29 | -8.667 | -1.009 | 12.122 | 1.00 | 0.00 |
| ATOM | 281 | N LBN | 18 | 0.656 | -5.110 | 5.504 | 1.00 | 0.00 | ATOM | 469 | CB LBN | 29 | -9.714 | -0.341 | 15.809 | 1.00 | 0.00 |
| ATOM | 282 | HN LBN | 18 | 0.640 | -2.603 | 2.075 | 1.00 | 0.00 | ATOM | 470 | HG1 LBN | 29 | -7.180 | -0.500 | 15.445 | 1.00 | 0.00 |
| ATOM | 283 | HA LBN | 18 | 0.575 | -6.377 | 6.514 | 1.00 | 0.00 | ATOM | 471 | HG2 LBN | 29 | -6.929 | -1.021 | 16.203 | 1.00 | 0.00 |
| ATOM | 284 | HA LBN | 18 | 0.546 | -6.995 | 6.358 | 1.00 | 0.00 | ATOM | 472 | CD LBN | 29 | -8.622 | -0.000 | 6.953 | 1.00 | 0.00 |
| ATOM | 285 | CB LBN | 18 | 0.629 | -7.225 | 6.155 | 1.00 | 0.00 | ATOM | 473 | CI LBN | 29 | -8.354 | -0.224 | 18.047 | 1.00 | 0.00 |
| ATOM | 286 | HBL LBN | 19 | 0.582 | -7.243 | 5.674 | 1.00 | 0.00 | ATOM | 474 | CR LBN | 29 | -8.371 | 1.007 | 14.688 | 1.00 | 0.00 |
| ATOM | 287 | HBL LBN | 19 | 0.748 | -8.897 | 1.000 | 1.00 | 0.00 | ATOM | 475 | CBR LBN | 29 | -1.053 | -0.995 | 12.267 | 1.00 | 0.00 |
| ATOM | 288 | CG LYS | 19 | 0.933 | -6.922 | 7.669 | 1.00 | 0.00 | ATOM | 476 | HG2 SER | 30 | -8.013 | -0.995 | 12.267 | 1.00 | 0.00 |
| ATOM | 289 | HG1 LYS | 19 | 0.693 | -7.018 | 8.633 | 1.00 | 0.00 | ATOM | 477 | CG SER | 30 | -9.714 | -0.341 | 15.809 | 1.00 | 0.00 |
| ATOM | 290 | HG2 LYS | 19 | 0.906 | -5.653 | 7.608 | 1.00 | 0.00 | ATOM | 478 | HG2 SER | 30 | -9.714 | -0.341 | 15.809 | 1.00 | 0.00 |
| ATOM | 291 | HA LYS | 19 | 0.412 | -7.319 | 7.429 | 1.00 | 0.00 | ATOM | 479 | CS SER | 30 | -7.871 | -1.000 | 11.111 | 1.00 | 0.00 |
| ATOM | 292 | HDI LYS | 19 | 1.012 | -7.444 | 6.365 | 1.00 | 0.00 | ATOM | 480 | OB SER | 30 | -8.056 | -1.562 | 1.611 | 1.00 | 0.00 |
| ATOM | 293 | HDI LYS | 19 | 1.156 | -7.592 | 7.823 | 1.00 | 0.00 | ATOM | 481 | NI ALA | 31 | -9.149 | -2.199 | 9.989 | 1.00 | 0.00 |
| ATOM | 294 | CE LYS | 19 | 1.067 | -6.671 | 7.506 | 1.00 | 0.00 | ATOM | 482 | HN ALA | 31 | -6.887 | -0.224 | 12.267 | 1.00 | 0.00 |
| ATOM | 295 | HE1 LYS | 19 | 0.987 | -9.401 | 7.506 | 1.00 | 0.00 | ATOM | 483 | HA ALA | 31 | -6.726 | -0.881 | 12.267 | 1.00 | 0.00 |
| ATOM | 296 | HE2 LYS | 19 | 10.988 | -9.598 | 9.117 | 1.00 | 0.00 | ATOM | 484 | HA ALA | 31 | -6.413 | -0.246 | 12.267 | 1.00 | 0.00 |
| ATOM | 297 | NZ LYS | 19 | 11.988 | -9.115 | 9.116 | 1.00 | 0.00 | ATOM | 485 | CB ALA | 31 | -6.553 | -1.712 | 12.267 | 1.00 | 0.00 |
| ATOM | 298 | HDI LYS | 19 | 12.044 | -10.147 | 10.141 | 1.00 | 0.00 | ATOM | 486 | HEL ALA | 31 | -6.226 | -0.246 | 12.267 | 1.00 | 0.00 |
| ATOM | 299 | HDI LYS | 19 | 12.418 | -8.955 | 9.057 | 1.00 | 0.00 | ATOM | 487 | HBL ALA | 31 | -7.743 | -1.184 | 7.740 | 1.00 | 0.00 |
| ATOM | 300 | HDI LYS | 19 | 12.526 | -8.661 | 9.280 | 1.00 | 0.00 | ATOM | 488 | HB1 ALA | 31 | -7.743 | -1.184 | 7.740 | 1.00 | 0.00 |
| ATOM | 301 | C LYS | 19 | 13.177 | -1.354 | 2.277 | 1.00 | 0.00 | ATOM | 489 | CH1 ALA | 31 | -7.006 | -1.736 | 7.433 | 1.00 | 0.00 |
| ATOM | 302 | O LYS | 19 | 13.198 | -1.354 | 2.277 | 1.00 | 0.00 | ATOM | 490 | O ALA | 31 | -7.745 | -1.590 | 8.860 | 1.00 | 0.00 |
| ATOM | 303 | N LYS | 20 | 6.377 | -1.342 | 2.277 | 1.00 | 0.00 | ATOM | 491 | RD1 TRP | 32 | -1.000 | -0.885 | 12.267 | 1.00 | 0.00 |
| ATOM | 304 | SER | 20 | 4.988 | -3.752 | 5.026 | 1.00 | 0.00 | ATOM | 492 | RD2 TRP | 32 | -1.022 | -2.398 | 12.267 | 1.00 | 0.00 |
| ATOM | 305 | GLY | 20 | 4.851 | -2.311 | 5.403 | 1.00 | 0.00 | ATOM | 493 | CA TRP | 32 | -1.022 | -2.394 | 12.267 | 1.00 | 0.00 |
| ATOM | 306 | HA SER | 20 | 5.448 | -5.222 | 6.155 | 1.00 | 0.00 | ATOM | 494 | HA TRP | 32 | -1.060 | -0.000 | 12.267 | 1.00 | 0.00 |
| ATOM | 307 | HOA SER | 20 | 5.590 | -1.189 | 7.866 | 1.00 | 0.00 | ATOM | 495 | CB TRP | 32 | -1.070 | -0.000 | 12.267 | 1.00 | 0.00 |
| ATOM | 308 | HOB SER | 20 | 7.401 | -0.573 | 7.427 | 1.00 | 0.00 | ATOM | 496 | HBL TRP | 32 | -1.167 | -2.390 | 12.267 | 1.00 | 0.00 |
| ATOM | 309 | HO2 SER | 20 | 5.331 | -1.177 | 8.283 | 1.00 | 0.00 | ATOM | 497 | HE2 TRP | 32 | -1.249 | -2.307 | 12.267 | 1.00 | 0.00 |
| ATOM | 310 | OQ SER | 20 | 8.046 | -3.222 | 9.559 | 1.00 | 0.00 | ATOM | 498 | IG TRP | 32 | -1.164 | -0.566 | 12.267 | 1.00 | 0.00 |
| ATOM | 311 | HG SER | 20 | 7.552 | -1.322 | 6.846 | 1.00 | 0.00 | ATOM | 499 | RD2 TRP | 32 | -1.130 | -0.566 | 12.267 | 1.00 | 0.00 |
| ATOM | 312 | CIS SER | 21 | 4.056 | -1.364 | 5.846 | 1.00 | 0.00 | ATOM | 500 | RD1 TRP | 32 | -1.082 | -0.052 | 12.267 | 1.00 | 0.00 |
| ATOM | 313 | N LEB | 21 | 4.723 | -2.227 | 6.155 | 1.00 | 0.00 | ATOM | 501 | NE1 TRP | 32 | -1.022 | -2.394 | 12.267 | 1.00 | 0.00 |
| ATOM | 314 | C LEB | 21 | 4.130 | -0.573 | 7.427 | 1.00 | 0.00 | ATOM | 502 | NE2 TRP | 32 | -1.069 | -0.000 | 12.267 | 1.00 | 0.00 |
| ATOM | 315 | CA LEB | 21 | 3.498 | -1.385 | 7.420 | 1.00 | 0.00 | ATOM | 503 | HE1 TRP | 32 | -1.182 | -2.395 | 12.267 | 1.00 | 0.00 |
| ATOM | 316 | HA LEB | 21 | 3.520 | -0.644 | 6.935 | 1.00 | 0.00 | ATOM | 504 | CE2 TRP | 32 | -1.167 | -2.390 | 12.267 | 1.00 | 0.00 |
| ATOM | 317 | HA LEB | 21 | 3.312 | -1.154 | 7.424 | 1.00 | 0.00 | ATOM | 505 | CE1 TRP | 32 | -1.279 | -2.307 | 12.267 | 1.00 | 0.00 |
| ATOM | 318 | CB LEB | 21 | 3.477 | -0.752 | 6.969 | 1.00 | 0.00 | ATOM | 506 | RD3 TRP | 32 | -1.164 | -0.566 | 12.267 | 1.00 | 0.00 |
| ATOM | 319 | HG LEB | 21 | 3.815 | -1.019 | 6.926 | 1.00 | 0.00 | ATOM | 507 | RD2 TRP | 32 | -1.271 | -1.026 | 12.267 | 1.00 | 0.00 |
| ATOM | 320 | OQ LEB | 21 | 4.155 | -1.364 | 5.846 | 1.00 | 0.00 | ATOM | 508 | RD1 TRP | 32 | -1.082 | -0.052 | 12.267 | 1.00 | 0.00 |
| ATOM | 321 | HO1 LEB | 21 | 4.289 | -1.022 | 4.568 | 1.00 | 0.00 | ATOM | 509 | SD2 TRP | 32 | -1.278 | -1.627 | 9.923 | 1.00 | 0.00 |
| ATOM | 322 | HO2 LEB | 21 | 4.772 | -2.227 | 6.155 | 1.00 | 0.00 | ATOM | 510 | SD1 TRP | 32 | -1.671 | -0.027 | 4.899 | 1.00 | 0.00 |
| ATOM | 323 | CIS LEB | 21 | 4.130 | -0.573 | 7.427 | 1.00 | 0.00 | ATOM | 511 | OB2 TRP | 32 | -1.244 | -2.395 | 12.267 | 1.00 | 0.00 |
| ATOM | 324 | | | | | | | | | | | | | | | | |

REPLACEMENT SHEET

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|------|-----|------|-----|----|---------|---------|--------|------|------|
| ATOM | 517 | CIO | PHE | 34 | -6.997 | 0.794 | 3.361 | 1.00 | 0.00 |
| ATOM | 518 | CDI | PHE | 34 | -7.638 | 0.503 | 2.562 | 1.00 | 0.00 |
| ATOM | 519 | COP | PHE | 34 | -5.300 | 0.255 | 4.946 | 1.00 | 0.00 |
| ATOM | 520 | PHS | PHE | 34 | -4.611 | -0.459 | 5.373 | 1.00 | 0.00 |
| ATOM | 541 | CEI | PHE | 34 | -7.069 | 2.077 | 3.688 | 1.00 | 0.00 |
| ATOM | 542 | HEI | PHE | 34 | -7.761 | 2.789 | 3.443 | 1.00 | 0.00 |
| ATOM | 543 | CZ2 | PHE | 34 | -5.368 | 1.932 | 5.459 | 1.00 | 0.00 |
| ATOM | 544 | HE2 | PHE | 34 | -4.728 | 1.024 | 6.279 | 1.00 | 0.00 |
| ATOM | 545 | CZ2 | PHE | 34 | -6.252 | 2.450 | 6.021 | 1.00 | 0.00 |
| ATOM | 546 | HE2 | PHE | 34 | -6.304 | 3.152 | 5.314 | 1.00 | 0.00 |
| ATOM | 547 | C | PHE | 34 | -7.400 | -3.024 | 5.033 | 1.00 | 0.00 |
| ATOM | 548 | O | PHE | 34 | -7.293 | -4.349 | 2.085 | 1.00 | 0.00 |
| ATOM | 549 | N | PHE | 35 | -7.543 | -4.100 | 2.285 | 1.00 | 0.00 |
| ATOM | 550 | NET | PHE | 35 | -6.635 | -3.476 | 5.035 | 1.00 | 0.00 |
| ATOM | 551 | CA | PHE | 35 | -7.387 | 5.592 | 5.541 | 1.00 | 0.00 |
| ATOM | 552 | HA | PHE | 35 | -6.624 | 5.946 | 5.223 | 1.00 | 0.00 |
| ATOM | 553 | HB | PHE | 35 | -7.660 | 5.808 | 6.023 | 1.00 | 0.00 |
| ATOM | 554 | HE2 | PHE | 35 | -6.472 | 4.598 | 6.413 | 1.00 | 0.00 |
| ATOM | 555 | HE2 | PHE | 35 | -6.605 | 6.119 | 6.850 | 1.00 | 0.00 |
| ATOM | 556 | COT | PHE | 35 | -6.620 | 5.387 | 6.288 | 1.00 | 0.00 |
| ATOM | 557 | NET | PHE | 35 | -6.714 | 5.337 | 6.279 | 1.00 | 0.00 |
| ATOM | 558 | HE2 | PHE | 35 | -5.766 | 7.589 | 7.437 | 1.00 | 0.00 |
| ATOM | 559 | SD | PHE | 35 | -6.296 | 7.590 | 7.242 | 1.00 | 0.00 |
| ATOM | 560 | CE | PHE | 35 | -6.148 | 8.011 | 6.470 | 1.00 | 0.00 |
| ATOM | 561 | HE1 | PHE | 35 | -4.744 | 8.722 | 7.013 | 1.00 | 0.00 |
| ATOM | 562 | HE2 | PHE | 35 | -4.668 | 8.724 | 7.013 | 1.00 | 0.00 |
| ATOM | 563 | HE3 | PHE | 35 | -5.157 | -6.114 | 5.529 | 1.00 | 0.00 |
| ATOM | 564 | C | PHE | 35 | -6.656 | -6.194 | 5.674 | 1.00 | 0.00 |
| ATOM | 565 | O | PHE | 35 | -6.847 | -5.924 | 3.827 | 1.00 | 0.00 |
| ATOM | 566 | N | PHE | 36 | -6.219 | -7.044 | 2.751 | 1.00 | 0.00 |
| ATOM | 567 | HRN | PHE | 36 | -7.255 | -7.708 | 2.671 | 1.00 | 0.00 |
| ATOM | 568 | CA | PHE | 36 | -9.128 | -7.792 | 7.020 | 1.00 | 0.00 |
| ATOM | 569 | HA | PHE | 36 | -5.598 | -8.566 | 4.149 | 1.00 | 0.00 |
| ATOM | 570 | CB | PHE | 36 | -11.371 | -8.248 | 2.562 | 1.00 | 0.00 |
| ATOM | 571 | HB1 | PHE | 36 | -11.151 | -7.501 | 2.496 | 1.00 | 0.00 |
| ATOM | 572 | HB2 | PHE | 36 | -10.122 | -8.460 | 3.601 | 1.00 | 0.00 |
| ATOM | 573 | CD | PHE | 36 | -10.307 | -9.553 | 1.996 | 1.00 | 0.00 |
| ATOM | 574 | HE1 | PHE | 36 | -10.073 | -10.933 | 1.748 | 1.00 | 0.00 |
| ATOM | 575 | HR2 | PHE | 36 | -11.473 | -8.138 | 1.102 | 1.00 | 0.00 |
| ATOM | 576 | CD | PHE | 36 | -11.006 | -10.289 | 2.972 | 1.00 | 0.00 |
| ATOM | 577 | OB1 | PHE | 36 | -11.522 | -11.463 | 3.266 | 1.00 | 0.00 |
| ATOM | 578 | OB2 | PHE | 36 | -12.794 | -9.685 | 3.440 | 1.00 | 0.00 |
| ATOM | 579 | C | PHE | 36 | -9.943 | -6.792 | 0.656 | 1.00 | 0.00 |
| ATOM | 580 | O | PHE | 36 | -10.414 | -5.939 | 0.873 | 1.00 | 0.00 |
| ATOM | 581 | N | PHE | 37 | -8.913 | -6.329 | -0.486 | 1.00 | 0.00 |
| ATOM | 582 | CA | PHE | 37 | -9.200 | -6.079 | -1.644 | 1.00 | 0.00 |
| ATOM | 583 | HA | PHE | 37 | -9.135 | -5.209 | -1.386 | 1.00 | 0.00 |
| ATOM | 584 | CB | PHE | 37 | -8.878 | -6.425 | -2.646 | 1.00 | 0.00 |
| ATOM | 585 | HE1 | PHE | 37 | -7.850 | -5.515 | -3.031 | 1.00 | 0.00 |
| ATOM | 586 | HE2 | PHE | 37 | -7.850 | -5.515 | -3.031 | 1.00 | 0.00 |
| ATOM | 587 | CD | PHE | 37 | -7.087 | -4.224 | -1.876 | 1.00 | 0.00 |
| ATOM | 588 | HE1 | PHE | 37 | -6.627 | -3.957 | -2.592 | 1.00 | 0.00 |
| ATOM | 589 | HE2 | PHE | 37 | -6.338 | -3.957 | -2.592 | 1.00 | 0.00 |
| ATOM | 590 | CO | PHE | 37 | -6.570 | -4.495 | 1.00 | 0.00 | 0.00 |
| ATOM | 591 | HE1 | PHE | 37 | -7.057 | -4.229 | 0.971 | 1.00 | 0.00 |
| ATOM | 592 | HE2 | PHE | 37 | -7.229 | -4.229 | 0.971 | 1.00 | 0.00 |
| ATOM | 593 | O | PHE | 37 | -6.276 | -4.934 | 1.137 | 1.00 | 0.00 |
| ATOM | 594 | CB | PHE | 37 | -10.861 | -10.289 | 2.972 | 1.00 | 0.00 |
| ATOM | 595 | HE1 | PHE | 37 | -11.522 | -11.463 | 3.266 | 1.00 | 0.00 |
| ATOM | 596 | HE2 | PHE | 37 | -11.522 | -11.463 | 3.266 | 1.00 | 0.00 |
| ATOM | 597 | CD | PHE | 37 | -11.000 | -10.289 | 2.972 | 1.00 | 0.00 |
| ATOM | 598 | OB1 | PHE | 37 | -11.779 | -10.289 | 2.972 | 1.00 | 0.00 |
| ATOM | 599 | OB2 | PHE | 37 | -11.779 | -10.289 | 2.972 | 1.00 | 0.00 |
| ATOM | 600 | HB | PHE | 38 | -11.233 | -9.585 | -5.534 | 1.00 | 0.00 |
| ATOM | 601 | CG1 | PHE | 38 | -11.202 | -3.977 | -5.534 | 1.00 | 0.00 |
| ATOM | 602 | HE11 | PHE | 38 | -12.102 | -3.610 | -5.211 | 1.00 | 0.00 |
| ATOM | 603 | HE12 | PHE | 38 | -10.644 | -3.864 | -5.171 | 1.00 | 0.00 |
| ATOM | 604 | HE21 | PHE | 38 | -12.250 | -3.628 | -4.479 | 1.00 | 0.00 |
| ATOM | 605 | CG2 | PHE | 38 | -11.677 | -4.229 | -5.208 | 1.00 | 0.00 |
| ATOM | 606 | HE22 | PHE | 38 | -11.433 | -6.633 | -5.266 | 1.00 | 0.00 |
| ATOM | 607 | HE23 | PHE | 38 | -11.433 | -4.933 | -7.070 | 1.00 | 0.00 |
| ATOM | 608 | HE23 | PHE | 38 | -14.998 | -9.319 | -4.047 | 1.00 | 0.00 |
| ATOM | 609 | CB | PHE | 38 | -14.855 | -9.995 | -4.546 | 1.00 | 0.00 |
| ATOM | 610 | HE1 | PHE | 38 | -12.222 | -7.700 | -4.513 | 1.00 | 0.00 |
| ATOM | 611 | HN | PHE | 38 | -14.615 | -10.931 | -3.727 | 1.00 | 0.00 |
| ATOM | 612 | HRN | PHE | 38 | -14.615 | -8.498 | -4.492 | 1.00 | 0.00 |
| ATOM | 613 | CA | PHE | 39 | -13.477 | -8.047 | -4.775 | 1.00 | 0.00 |
| ATOM | 614 | HE1 | PHE | 39 | -14.173 | -7.357 | -4.773 | 1.00 | 0.00 |
| ATOM | 615 | HE2 | PHE | 39 | -13.450 | -8.431 | -5.053 | 1.00 | 0.00 |
| ATOM | 616 | CA | PHE | 39 | -13.050 | -8.431 | -5.053 | 1.00 | 0.00 |
| ATOM | 617 | HE1 | PHE | 39 | -12.960 | -10.935 | -4.968 | 1.00 | 0.00 |
| ATOM | 618 | HE2 | PHE | 39 | -14.498 | -8.024 | -6.071 | 1.00 | 0.00 |
| ATOM | 619 | CB | PHE | 39 | -14.640 | -10.935 | -4.968 | 1.00 | 0.00 |
| ATOM | 620 | HE1 | PHE | 39 | -14.640 | -10.935 | -4.968 | 1.00 | 0.00 |
| ATOM | 621 | CD | PHE | 39 | -14.283 | -9.316 | -5.209 | 1.00 | 0.00 |
| ATOM | 622 | HO1 | PHE | 39 | -17.164 | -8.759 | -5.263 | 1.00 | 0.00 |
| ATOM | 623 | HO2 | PHE | 39 | -16.460 | -10.357 | -2.664 | 1.00 | 0.00 |
| ATOM | 624 | CG | PHE | 39 | -16.415 | -8.024 | -6.071 | 1.00 | 0.00 |
| ATOM | 625 | HE1 | PHE | 39 | -15.855 | -9.316 | -5.053 | 1.00 | 0.00 |
| ATOM | 626 | HE2 | PHE | 39 | -15.855 | -9.316 | -5.053 | 1.00 | 0.00 |
| ATOM | 627 | CD | PHE | 39 | -14.985 | -8.065 | -6.071 | 1.00 | 0.00 |
| ATOM | 628 | HO1 | PHE | 39 | -14.985 | -8.065 | -6.071 | 1.00 | 0.00 |
| ATOM | 629 | HO2 | PHE | 39 | -14.985 | -8.065 | -6.071 | 1.00 | 0.00 |
| ATOM | 630 | CD | PHE | 39 | -14.985 | -8.065 | -6.071 | 1.00 | 0.00 |
| ATOM | 631 | CA | LYS | 39 | -14.985 | -8.033 | -5.056 | 1.00 | 0.00 |
| ATOM | 632 | CB | LYS | 39 | -14.985 | -8.033 | -5.056 | 1.00 | 0.00 |
| ATOM | 633 | CD | LYS | 39 | -14.985 | -8.033 | -5.056 | 1.00 | 0.00 |
| ATOM | 634 | HE1 | LYS | 39 | -14.985 | -8.033 | -5.056 | 1.00 | 0.00 |
| ATOM | 635 | HE2 | LYS | 39 | -14.985 | -8.033 | -5.056 | 1.00 | 0.00 |
| ATOM | 636 | CD | PHE | 39 | -14.611 | -8.033 | -5.056 | 1.00 | 0.00 |
| ATOM | 637 | CB | PHE | 39 | -14.611 | -8.033 | -5.056 | 1.00 | 0.00 |
| ATOM | 638 | CD | PHE | 39 | -14.611 | -8.033 | -5.056 | 1.00 | 0.00 |
| ATOM | 639 | CB | PHE | 39 | -14.611 | -8.033 | -5.056 | 1.00 | 0.00 |
| ATOM | 640 | CD | PHE | 39 | -14.611 | -8.033 | -5.056 | 1.00 | 0.00 |
| ATOM | 641 | CB | PHE | 39 | -14.611 | -8.033 | -5.056 | 1.00 | 0.00 |
| ATOM | 642 | CD | PHE | 39 | -14.611 | -8.033 | -5.056 | 1.00 | 0.00 |
| ATOM | 643 | CB | PHE | 39 | -14.611 | -8.033 | -5.056 | 1.00 | 0.00 |
| ATOM | 644 | CD | PHE | 39 | -14.611 | -8.033 | -5.056 | 1.00 | 0.00 |
| ATOM | 645 | CB | PHE | 39 | -14.611 | -8.033 | -5.056 | 1.00 | 0.00 |
| ATOM | 646 | CD | PHE | 39 | -14.611 | -8.033 | -5.056 | 1.00 | 0.00 |
| ATOM | 647 | CB | PHE | 39 | -14.611 | -8.033 | -5.056 | 1.00 | 0.00 |
| ATOM | 648 | CD | PHE | 39 | -14.611 | -8.033 | -5.056 | 1.00 | 0.00 |
| ATOM | 649 | CB | PHE | 39 | -14.611 | -8.033 | -5.056 | 1.00 | 0.00 |
| ATOM | 650 | CD | PHE | 39 | -14.611 | -8.033 | -5.056 | 1.00 | 0.00 |
| ATOM | 651 | CB | PHE | 39 | -14.611 | -8.033 | -5.056 | 1.00 | 0.00 |
| ATOM | 652 | CD | PHE | 39 | -14.611 | -8.033 | -5.056 | 1.00 | 0.00 |
| ATOM | 653 | CB | PHE | 39 | -14.611 | -8.033 | -5.056 | 1.00 | 0.00 |
| ATOM | 654 | CD | PHE | 39 | -14.611 | -8.033 | -5.056 | 1.00 | 0.00 |
| ATOM | 655 | CB | PHE | 39 | -14.611 | -8.033 | -5.056 | 1.00 | 0.00 |
| ATOM | 656 | CD | PHE | 39 | -14.611 | -8.033 | -5.056 | 1.00 | 0.00 |
| ATOM | 657 | CB | PHE | 39 | -14.611 | -8.033 | -5.056 | 1.00 | 0.00 |
| ATOM | 658 | CD | PHE | 39 | -14.611 | -8.033 | -5.056 | 1.00 | 0.00 |
| ATOM | 659 | CB | PHE | 39 | -14.611 | -8.033 | -5.056 | 1.00 | 0.00 |
| ATOM | 660 | CD | PHE | 39 | -14.611 | -8.033 | -5.056 | 1.00 | 0.00 |
| ATOM | 661 | CB | PHE | 39 | -14.611 | -8.033 | -5.056 | 1.00 | 0.00 |
| ATOM | 662 | CD | PHE | 39 | -14.611 | -8.033 | -5.056 | 1.00 | 0.00 |
| ATOM | 663 | CB | PHE | 39 | -14.611 | -8.033 | -5.056 | 1.00 | 0.00 |
| ATOM | 664 | CD | PHE | 39 | -14.611 | -8.033 | -5.056 | 1.00 | 0.00 |
| ATOM | 665 | CB | PHE | | | | | | |

REPLACEMENT SHEET

| | | | | | | | | |
|------|-----|----------|----|--------|--------|---------|------|------|
| ATOM | 819 | CD ARG | 51 | -2.433 | 4.849 | -11.240 | 1.00 | 0.00 |
| ATOM | 820 | HDL ARG | 51 | -2.996 | 5.010 | -10.332 | 1.00 | 0.00 |
| ATOM | 821 | HDL ARG | 51 | -1.566 | 5.493 | -11.244 | 1.00 | 0.00 |
| ATOM | 822 | HDL ARG | 51 | -3.275 | 5.184 | -12.395 | 1.00 | 0.00 |
| ATOM | 823 | HE ARG | 51 | -4.217 | 5.390 | -12.212 | 1.00 | 0.00 |
| ATOM | 824 | HE ARG | 51 | -2.832 | 5.256 | -13.688 | 1.00 | 0.00 |
| ATOM | 825 | HHL ARG | 51 | -1.582 | 4.983 | -13.904 | 1.00 | 0.00 |
| ATOM | 826 | HHL ARG | 51 | -1.231 | 4.984 | -14.866 | 1.00 | 0.00 |
| ATOM | 827 | HHL ARG | 51 | -0.936 | 4.716 | -13.161 | 1.00 | 0.00 |
| ATOM | 828 | HHL ARG | 51 | -3.659 | 5.519 | -14.666 | 1.00 | 0.00 |
| ATOM | 829 | HHL ARG | 51 | -3.273 | 5.599 | -15.588 | 1.00 | 0.00 |
| ATOM | 830 | HHL ARG | 51 | -4.617 | 5.766 | -14.460 | 1.00 | 0.00 |
| ATOM | 831 | C ARG | 51 | -4.084 | 5.134 | -11.066 | 1.00 | 0.00 |
| ATOM | 832 | O ARG | 51 | -4.094 | 0.319 | -12.061 | 1.00 | 0.00 |
| ATOM | 833 | SER | 52 | -3.479 | -0.122 | -9.901 | 1.00 | 0.00 |
| ATOM | 834 | IN SER | 52 | -3.170 | 0.463 | -9.184 | 1.00 | 0.00 |
| ATOM | 835 | HA SER | 52 | -3.166 | 1.623 | -7.731 | 1.00 | 0.00 |
| ATOM | 836 | CA SER | 52 | -3.166 | 2.171 | -7.731 | 1.00 | 0.00 |
| ATOM | 837 | CB SER | 52 | -3.160 | 1.980 | -9.755 | 1.00 | 0.00 |
| ATOM | 838 | CG SER | 52 | -1.650 | 1.980 | -9.755 | 1.00 | 0.00 |
| ATOM | 839 | HB1 SER | 52 | -1.447 | 1.890 | -9.758 | 1.00 | 0.00 |
| ATOM | 840 | HB2 SER | 52 | -1.477 | 1.890 | -9.758 | 1.00 | 0.00 |
| ATOM | 841 | HG SER | 52 | -1.672 | -1.619 | -9.877 | 1.00 | 0.00 |
| ATOM | 842 | C SER | 52 | -3.993 | -2.118 | -9.488 | 1.00 | 0.00 |
| ATOM | 843 | O SER | 52 | -3.353 | -2.108 | -7.462 | 1.00 | 0.00 |
| ATOM | 844 | N PRO | 53 | -5.310 | -2.179 | -8.565 | 1.00 | 0.00 |
| ATOM | 845 | CA PRO | 53 | -5.307 | -2.882 | -7.455 | 1.00 | 0.00 |
| ATOM | 846 | HA PRO | 53 | -6.390 | -2.033 | -6.773 | 1.00 | 0.00 |
| ATOM | 847 | CB PRO | 53 | -6.176 | -1.577 | -6.060 | 1.00 | 0.00 |
| ATOM | 848 | CG PRO | 53 | -7.113 | -3.489 | -6.111 | 1.00 | 0.00 |
| ATOM | 849 | HB1 PRO | 53 | -5.455 | -3.145 | -7.450 | 1.00 | 0.00 |
| ATOM | 850 | HB2 PRO | 53 | -7.122 | -4.559 | -8.355 | 1.00 | 0.00 |
| ATOM | 851 | HGL PRO | 53 | -7.512 | -2.663 | -9.337 | 1.00 | 0.00 |
| ATOM | 852 | HGL PRO | 53 | -7.963 | -3.263 | -10.110 | 1.00 | 0.00 |
| ATOM | 853 | CD PRO | 53 | -8.139 | -1.812 | -9.510 | 1.00 | 0.00 |
| ATOM | 854 | HDL PRO | 53 | -5.780 | -2.805 | -10.584 | 1.00 | 0.00 |
| ATOM | 855 | HDL PRO | 53 | -6.176 | -1.157 | -10.060 | 1.00 | 0.00 |
| ATOM | 856 | C PRO | 53 | -5.340 | -3.947 | -6.639 | 1.00 | 0.00 |
| ATOM | 857 | O PRO | 53 | -4.455 | -5.137 | -6.943 | 1.00 | 0.00 |
| ATOM | 858 | N MET | 54 | -4.649 | -3.512 | -5.619 | 1.00 | 0.00 |
| ATOM | 859 | HE MET | 54 | -4.591 | -3.522 | -5.456 | 1.00 | 0.00 |
| ATOM | 860 | CA MET | 54 | -3.850 | -4.428 | -4.777 | 1.00 | 0.00 |
| ATOM | 861 | HA MET | 54 | -4.303 | -5.405 | -4.859 | 1.00 | 0.00 |
| ATOM | 862 | CB MET | 54 | -2.98 | -4.508 | -5.253 | 1.00 | 0.00 |
| ATOM | 863 | HB1 MET | 54 | -2.390 | -4.624 | -5.287 | 1.00 | 0.00 |
| ATOM | 864 | HB2 MET | 54 | -1.897 | -3.587 | -4.995 | 1.00 | 0.00 |
| ATOM | 865 | CG MET | 54 | -1.615 | -5.660 | -4.644 | 1.00 | 0.00 |
| ATOM | 866 | HDL MET | 54 | -1.472 | -5.464 | -3.592 | 1.00 | 0.00 |
| ATOM | 867 | CD MET | 54 | -0.653 | -5.122 | -5.122 | 1.00 | 0.00 |
| ATOM | 868 | HE MET | 54 | -2.452 | -7.247 | -4.826 | 1.00 | 0.00 |
| ATOM | 869 | NE MET | 54 | -3.383 | -7.311 | -3.288 | 1.00 | 0.00 |
| ATOM | 870 | HEI MET | 54 | -2.405 | -7.997 | -2.612 | 1.00 | 0.00 |
| ATOM | 871 | HEZ MET | 54 | -4.308 | -6.650 | -1.650 | 1.00 | 0.00 |
| ATOM | 872 | HEZ MET | 54 | -3.418 | -6.277 | -2.857 | 1.00 | 0.00 |
| ATOM | 873 | O MET | 54 | -3.897 | -3.294 | -3.294 | 1.00 | 0.00 |
| ATOM | 874 | O MET | 54 | -2.327 | -4.445 | -2.802 | 1.00 | 0.00 |
| ATOM | 875 | O MET | 54 | -1.472 | -5.464 | -3.592 | 1.00 | 0.00 |
| ATOM | 876 | IN MET | 54 | -0.653 | -5.122 | -5.122 | 1.00 | 0.00 |
| ATOM | 877 | CA ASP | 55 | -3.870 | -3.870 | -3.870 | 1.00 | 0.00 |
| ATOM | 878 | HA ASP | 55 | -4.603 | -2.874 | -1.119 | 1.00 | 0.00 |
| ATOM | 879 | CB ASP | 55 | -4.690 | -3.863 | -0.916 | 1.00 | 0.00 |
| ATOM | 880 | HB1 ASP | 55 | -6.811 | -0.102 | -0.102 | 1.00 | 0.00 |
| ATOM | 881 | HB2 ASP | 55 | -7.075 | -4.865 | -0.944 | 1.00 | 0.00 |
| ATOM | 882 | CG ASP | 55 | -7.075 | -2.885 | -0.815 | 1.00 | 0.00 |
| ATOM | 883 | OD1 ASP | 55 | -7.575 | -3.041 | -0.010 | 1.00 | 0.00 |
| ATOM | 884 | OD2 ASP | 55 | -8.074 | -1.881 | -0.010 | 1.00 | 0.00 |
| ATOM | 885 | C ASP | 55 | -4.435 | -4.826 | -3.626 | 1.00 | 0.00 |
| ATOM | 886 | O ASP | 55 | -4.378 | -5.778 | -5.580 | 1.00 | 0.00 |
| ATOM | 887 | N LEU | 56 | -4.739 | -4.786 | -0.919 | 1.00 | 0.00 |
| ATOM | 888 | HN LEU | 56 | -5.426 | -4.165 | -2.242 | 1.00 | 0.00 |
| ATOM | 889 | CA LEU | 56 | -4.069 | -5.640 | -1.688 | 1.00 | 0.00 |
| ATOM | 890 | HA LEU | 56 | -4.012 | -5.620 | -1.681 | 1.00 | 0.00 |
| ATOM | 891 | CB LEU | 56 | -4.205 | -5.115 | -3.108 | 1.00 | 0.00 |
| ATOM | 892 | HB1 LEU | 56 | -4.223 | -2.352 | -2.352 | 1.00 | 0.00 |
| ATOM | 893 | HB2 LEU | 56 | -1.929 | -4.584 | -3.801 | 1.00 | 0.00 |
| ATOM | 894 | HEI LEU | 56 | -1.779 | -3.291 | -3.291 | 1.00 | 0.00 |
| ATOM | 895 | HEZ LEU | 56 | -3.343 | -4.015 | -3.377 | 1.00 | 0.00 |
| ATOM | 896 | NE LEU | 56 | -3.605 | -3.702 | -4.770 | 1.00 | 0.00 |
| ATOM | 897 | HD1 LEU | 56 | -4.611 | -4.656 | -4.824 | 1.00 | 0.00 |
| ATOM | 898 | HD2 LEU | 56 | -4.668 | -1.773 | -1.000 | 1.00 | 0.00 |
| ATOM | 899 | HD3 LEU | 56 | -3.425 | -2.802 | -2.859 | 1.00 | 0.00 |
| ATOM | 900 | HD4 LEU | 56 | -3.604 | -1.924 | -3.449 | 1.00 | 0.00 |
| ATOM | 901 | HD5 LEU | 56 | -4.204 | -2.255 | -2.132 | 1.00 | 0.00 |
| ATOM | 902 | HD6 LEU | 56 | -4.281 | -2.188 | -2.352 | 1.00 | 0.00 |
| ATOM | 903 | HD7 LEU | 56 | -4.253 | -3.371 | -3.371 | 1.00 | 0.00 |
| ATOM | 904 | HD8 LEU | 56 | -4.631 | -1.706 | -1.000 | 1.00 | 0.00 |
| ATOM | 905 | HD9 LEU | 56 | -4.667 | -1.942 | -1.000 | 1.00 | 0.00 |
| ATOM | 906 | HD10 LEU | 56 | -4.262 | -2.162 | -2.162 | 1.00 | 0.00 |
| ATOM | 907 | HD11 LEU | 56 | -4.262 | -2.162 | -2.162 | 1.00 | 0.00 |
| ATOM | 908 | HD12 LEU | 56 | -4.262 | -2.162 | -2.162 | 1.00 | 0.00 |
| ATOM | 909 | HD13 LEU | 56 | -4.223 | -2.181 | -2.181 | 1.00 | 0.00 |
| ATOM | 910 | HD14 LEU | 56 | -4.223 | -2.181 | -2.181 | 1.00 | 0.00 |
| ATOM | 911 | HD15 LEU | 56 | -4.223 | -2.181 | -2.181 | 1.00 | 0.00 |
| ATOM | 912 | HD16 LEU | 56 | -4.223 | -2.181 | -2.181 | 1.00 | 0.00 |
| ATOM | 913 | HD17 LEU | 56 | -4.223 | -2.181 | -2.181 | 1.00 | 0.00 |
| ATOM | 914 | HD18 LEU | 56 | -4.223 | -2.181 | -2.181 | 1.00 | 0.00 |
| ATOM | 915 | HD19 LEU | 56 | -4.223 | -2.181 | -2.181 | 1.00 | 0.00 |
| ATOM | 916 | HD20 LEU | 56 | -4.223 | -2.181 | -2.181 | 1.00 | 0.00 |
| ATOM | 917 | HD21 LEU | 56 | -4.223 | -2.181 | -2.181 | 1.00 | 0.00 |
| ATOM | 918 | HD22 LEU | 56 | -4.223 | -2.181 | -2.181 | 1.00 | 0.00 |
| ATOM | 919 | HD23 LEU | 56 | -4.223 | -2.181 | -2.181 | 1.00 | 0.00 |
| ATOM | 920 | HD24 LEU | 56 | -4.223 | -2.181 | -2.181 | 1.00 | 0.00 |
| ATOM | 921 | HD25 LEU | 56 | -4.223 | -2.181 | -2.181 | 1.00 | 0.00 |
| ATOM | 922 | HD26 LEU | 56 | -4.223 | -2.181 | -2.181 | 1.00 | 0.00 |
| ATOM | 923 | HD27 LEU | 56 | -4.223 | -2.181 | -2.181 | 1.00 | 0.00 |
| ATOM | 924 | HD28 LEU | 56 | -4.223 | -2.181 | -2.181 | 1.00 | 0.00 |
| ATOM | 925 | HD29 LEU | 56 | -4.223 | -2.181 | -2.181 | 1.00 | 0.00 |
| ATOM | 926 | HD30 LEU | 56 | -4.223 | -2.181 | -2.181 | 1.00 | 0.00 |
| ATOM | 927 | HD31 LEU | 56 | -4.223 | -2.181 | -2.181 | 1.00 | 0.00 |
| ATOM | 928 | HD32 LEU | 56 | -4.223 | -2.181 | -2.181 | 1.00 | 0.00 |
| ATOM | 929 | HD33 LEU | 56 | -4.223 | -2.181 | -2.181 | 1.00 | 0.00 |
| ATOM | 930 | HD34 LEU | 56 | -4.223 | -2.181 | -2.181 | 1.00 | 0.00 |
| ATOM | 931 | CB LYS | 57 | -4.075 | -2.576 | -1.000 | 1.00 | 0.00 |
| ATOM | 932 | CD LYS | 57 | -4.075 | -2.576 | -1.000 | 1.00 | 0.00 |
| ATOM | 933 | CE LYS | 57 | -4.075 | -2.576 | -1.000 | 1.00 | 0.00 |
| ATOM | 934 | CE2 LYS | 57 | -4.075 | -2.576 | -1.000 | 1.00 | 0.00 |
| ATOM | 935 | CE3 LYS | 57 | -4.075 | -2.576 | -1.000 | 1.00 | 0.00 |
| ATOM | 936 | CE4 LYS | 57 | -4.075 | -2.576 | -1.000 | 1.00 | 0.00 |
| ATOM | 937 | CE5 LYS | 57 | -4.075 | -2.576 | -1.000 | 1.00 | 0.00 |
| ATOM | 938 | CE6 LYS | 57 | -4.075 | -2.576 | -1.000 | 1.00 | 0.00 |
| ATOM | 939 | CE7 LYS | 57 | -4.075 | -2.576 | -1.000 | 1.00 | 0.00 |
| ATOM | 940 | CE8 LYS | 57 | -4.075 | -2.576 | -1.000 | 1.00 | 0.00 |
| ATOM | 941 | CE9 LYS | 57 | -4.075 | -2.576 | -1.000 | 1.00 | 0.00 |
| ATOM | 942 | CE10 LYS | 57 | -4.075 | -2.576 | -1.000 | 1.00 | 0.00 |
| ATOM | 943 | CE11 LYS | 57 | -4.075 | -2.576 | -1.000 | 1.00 | 0.00 |
| ATOM | 944 | CE12 LYS | 57 | -4.075 | -2.576 | -1.000 | 1.00 | 0.00 |
| ATOM | 945 | CE13 LYS | 57 | -4.075 | -2.576 | -1.000 | 1.00 | 0.00 |
| ATOM | 946 | CE14 LYS | 57 | -4.075 | -2.576 | -1.000 | 1.00 | 0.00 |
| ATOM | 947 | CE15 LYS | 57 | -4.075 | -2.576 | -1.000 | 1.00 | 0.00 |
| ATOM | 948 | CE16 LYS | 57 | -4.075 | -2.576 | -1.000 | 1.00 | 0.00 |
| ATOM | 949 | CE17 LYS | 57 | -4.075 | -2.576 | -1.000 | 1.00 | 0.00 |
| ATOM | 950 | CE18 LYS | 57 | -4.075 | -2.576 | -1.000 | 1.00 | 0.00 |
| ATOM | 951 | CE19 LYS | 57 | -4.075 | -2.576 | -1.000 | 1.00 | 0.00 |
| ATOM | 952 | CE20 LYS | 57 | -4.075 | -2.576 | -1.000 | 1.00 | 0.00 |
| ATOM | 953 | CE21 LYS | 57 | -4.075 | -2.576 | -1.000 | 1.00 | 0.00 |
| ATOM | 954 | CE22 LYS | 57 | -4.075 | -2.576 | -1.000 | 1.00 | 0.00 |
| ATOM | | | | | | | | |

REPLACEMENT SHEET

| | | | | | | | | | |
|------|------|------|-----|----|--------|---------|---------|------|------|
| ATOM | 1101 | HEI | TIR | 67 | 6.089 | -16.237 | -6.940 | 1.00 | 0.00 |
| ATOM | 1102 | HEI | TIR | 67 | 6.098 | -13.133 | -7.044 | 1.00 | 0.00 |
| ATOM | 1103 | HEI | TIR | 67 | 6.081 | -12.449 | -7.711 | 1.00 | 0.00 |
| ATOM | 1104 | HEI | TIR | 67 | 5.952 | -13.497 | -7.466 | 1.00 | 0.00 |
| ATOM | 1105 | HEI | TIR | 67 | 5.930 | -14.793 | -8.745 | 1.00 | 0.00 |
| ATOM | 1106 | HEI | TIR | 67 | 5.926 | -15.205 | -8.737 | 1.00 | 0.00 |
| ATOM | 1107 | C | TIR | 67 | 5.966 | -10.880 | -3.889 | 1.00 | 0.00 |
| ATOM | 1108 | HEI | TIR | 67 | 5.990 | -10.653 | -5.063 | 1.00 | 0.00 |
| ATOM | 1109 | N | TIR | 68 | 6.059 | -9.977 | -2.953 | 1.00 | 0.00 |
| ATOM | 1110 | HEI | TIR | 68 | 6.099 | -10.817 | -1.988 | 1.00 | 0.00 |
| ATOM | 1111 | A | TIR | 68 | 6.515 | -6.568 | -3.200 | 1.00 | 0.00 |
| ATOM | 1112 | HEI | TIR | 68 | 6.570 | -6.455 | -4.355 | 1.00 | 0.00 |
| ATOM | 1113 | G | TIR | 68 | 6.509 | -6.283 | -2.821 | 1.00 | 0.00 |
| ATOM | 1114 | HEI | TIR | 68 | 6.446 | -6.005 | -2.266 | 1.00 | 0.00 |
| ATOM | 1115 | H | TIR | 68 | 6.466 | -6.146 | -2.266 | 1.00 | 0.00 |
| ATOM | 1116 | O | TIR | 68 | 6.489 | -6.173 | -3.966 | 1.00 | 0.00 |
| ATOM | 1117 | C | TIR | 68 | 6.479 | -6.173 | -5.514 | 1.00 | 0.00 |
| ATOM | 1118 | H | TIR | 68 | 6.577 | -6.173 | -5.314 | 1.00 | 0.00 |
| ATOM | 1119 | C | TIR | 68 | 6.546 | -6.173 | -5.314 | 1.00 | 0.00 |
| ATOM | 1120 | H | TIR | 68 | 6.583 | -6.173 | -5.314 | 1.00 | 0.00 |
| ATOM | 1121 | H | TIR | 68 | 6.578 | -6.173 | -5.314 | 1.00 | 0.00 |
| ATOM | 1122 | C | TIR | 68 | 6.569 | -6.173 | -5.314 | 1.00 | 0.00 |
| ATOM | 1123 | S | TIR | 68 | 6.359 | -6.568 | -6.196 | 1.00 | 0.00 |
| ATOM | 1124 | HEI | TIR | 68 | 6.323 | -6.975 | -7.143 | 1.00 | 0.00 |
| ATOM | 1125 | H | TIR | 68 | 6.202 | -6.781 | -4.765 | 1.00 | 0.00 |
| ATOM | 1126 | E | TIR | 68 | 6.141 | -6.581 | -4.633 | 1.00 | 0.00 |
| ATOM | 1127 | C | TIR | 68 | 6.233 | -7.811 | -5.998 | 1.00 | 0.00 |
| ATOM | 1128 | OH | TIR | 68 | 6.135 | -6.765 | -7.013 | 1.00 | 0.00 |
| ATOM | 1129 | H | TIR | 68 | 6.044 | -6.751 | -6.637 | 1.00 | 0.00 |
| ATOM | 1130 | N | TIR | 68 | 6.783 | -7.344 | -6.923 | 1.00 | 0.00 |
| ATOM | 1131 | HN | TIR | 68 | 6.395 | -6.844 | -6.923 | 1.00 | 0.00 |
| ATOM | 1132 | HN | TIR | 68 | 6.706 | -6.457 | -2.303 | 1.00 | 0.00 |
| ATOM | 1133 | N | TIR | 68 | 6.844 | -7.344 | -5.259 | 1.00 | 0.00 |
| ATOM | 1134 | HG12 | VAL | 69 | 9.000 | -8.862 | -2.835 | 1.00 | 0.00 |
| ATOM | 1135 | HG13 | VAL | 69 | 10.423 | -9.887 | -1.712 | 1.00 | 0.00 |
| ATOM | 1136 | HA | VAL | 69 | 9.761 | -10.795 | -1.962 | 1.00 | 0.00 |
| ATOM | 1137 | HN | VAL | 69 | 9.284 | -10.461 | -1.221 | 1.00 | 0.00 |
| ATOM | 1138 | CA | VAL | 69 | 10.907 | -7.375 | -1.276 | 1.00 | 0.00 |
| ATOM | 1139 | CB | VAL | 69 | 11.715 | -7.964 | -1.964 | 1.00 | 0.00 |
| ATOM | 1140 | CG | VAL | 69 | 10.655 | -8.242 | -0.846 | 1.00 | 0.00 |
| ATOM | 1141 | CD | VAL | 69 | 10.775 | -8.343 | -0.933 | 1.00 | 0.00 |
| ATOM | 1142 | CG | VAL | 69 | 11.171 | -8.640 | -1.133 | 1.00 | 0.00 |
| ATOM | 1143 | CA | VAL | 69 | 10.422 | -7.059 | -0.090 | 1.00 | 0.00 |
| ATOM | 1144 | HG22 | VAL | 69 | 11.977 | -6.979 | -0.411 | 1.00 | 0.00 |
| ATOM | 1145 | HG23 | VAL | 69 | 11.822 | -6.118 | -0.438 | 1.00 | 0.00 |
| ATOM | 1146 | O | VAL | 69 | 10.352 | -6.199 | -3.043 | 1.00 | 0.00 |
| ATOM | 1147 | O | VAL | 69 | 11.543 | -6.277 | -3.305 | 1.00 | 0.00 |
| ATOM | 1148 | HN | SER | 70 | 9.507 | -6.372 | -3.634 | 1.00 | 0.00 |
| ATOM | 1149 | HN | SER | 70 | 8.566 | -5.371 | -3.359 | 1.00 | 0.00 |
| ATOM | 1150 | CG | SER | 70 | 9.934 | -4.491 | -4.703 | 1.00 | 0.00 |
| ATOM | 1151 | CB | SER | 70 | 10.985 | -4.486 | -4.000 | 1.00 | 0.00 |
| ATOM | 1152 | HEI | SER | 70 | 10.826 | -4.569 | -5.161 | 1.00 | 0.00 |
| ATOM | 1153 | HEI | SER | 70 | 9.476 | -4.253 | -4.253 | 1.00 | 0.00 |
| ATOM | 1154 | HG | SER | 70 | 10.775 | -4.300 | -4.600 | 1.00 | 0.00 |
| ATOM | 1155 | O | SER | 70 | 10.674 | -4.164 | -4.677 | 1.00 | 0.00 |
| ATOM | 1156 | O | SER | 70 | 9.656 | -4.177 | -4.677 | 1.00 | 0.00 |
| ATOM | 1157 | N | SER | 70 | 9.769 | -4.159 | -4.249 | 1.00 | 0.00 |
| ATOM | 1158 | CA | VAL | 70 | 10.985 | -4.267 | -4.582 | 1.00 | 0.00 |
| ATOM | 1159 | CA | VAL | 71 | 10.812 | -4.267 | -4.582 | 1.00 | 0.00 |
| ATOM | 1160 | CA | VAL | 71 | 9.858 | -4.267 | -4.582 | 1.00 | 0.00 |
| ATOM | 1161 | CA | VAL | 71 | 10.879 | -4.267 | -4.582 | 1.00 | 0.00 |
| ATOM | 1162 | HB1 | VAL | 71 | 10.771 | -4.267 | -4.582 | 1.00 | 0.00 |
| ATOM | 1163 | HB2 | VAL | 71 | 10.771 | -4.267 | -4.582 | 1.00 | 0.00 |
| ATOM | 1164 | CG | VAL | 71 | 9.656 | -4.267 | -4.582 | 1.00 | 0.00 |
| ATOM | 1165 | HG1 | VAL | 71 | 9.554 | -4.267 | -4.582 | 1.00 | 0.00 |
| ATOM | 1166 | HG2 | VAL | 71 | 10.506 | -4.267 | -4.582 | 1.00 | 0.00 |
| ATOM | 1167 | CD | VAL | 71 | 10.218 | -4.233 | -4.582 | 1.00 | 0.00 |
| ATOM | 1168 | HD1 | VAL | 71 | 11.031 | -4.663 | -5.631 | 1.00 | 0.00 |
| ATOM | 1169 | HD2 | VAL | 71 | 9.424 | -4.233 | -4.582 | 1.00 | 0.00 |
| ATOM | 1170 | CD | VAL | 71 | 10.721 | -4.321 | -4.582 | 1.00 | 0.00 |
| ATOM | 1171 | HE1 | VAL | 71 | 11.466 | -3.737 | -5.506 | 1.00 | 0.00 |
| ATOM | 1172 | HE2 | VAL | 71 | 9.891 | -4.412 | -5.119 | 1.00 | 0.00 |
| ATOM | 1173 | HE3 | VAL | 71 | 11.323 | -4.511 | -5.477 | 1.00 | 0.00 |
| ATOM | 1174 | HE1 | VAL | 71 | 10.580 | -4.970 | -8.021 | 1.00 | 0.00 |
| ATOM | 1175 | HE2 | VAL | 71 | 11.823 | -3.822 | -8.056 | 1.00 | 0.00 |
| ATOM | 1176 | HE3 | VAL | 71 | 12.000 | -5.234 | -7.344 | 1.00 | 0.00 |
| ATOM | 1177 | C | VAL | 71 | 7.984 | -6.678 | -7.344 | 1.00 | 0.00 |
| ATOM | 1178 | O | VAL | 71 | 8.016 | -6.678 | -7.344 | 1.00 | 0.00 |
| ATOM | 1179 | N | VAL | 72 | 10.721 | -3.024 | -6.564 | 1.00 | 0.00 |
| ATOM | 1180 | HN | VAL | 72 | 9.002 | -0.018 | -6.730 | 1.00 | 0.00 |
| ATOM | 1181 | CA | VAL | 72 | 6.963 | -0.053 | -7.86 | 1.00 | 0.00 |
| ATOM | 1182 | HA | VAL | 72 | 6.511 | -0.053 | -7.86 | 1.00 | 0.00 |
| ATOM | 1183 | CB | VAL | 72 | 11.876 | -2.028 | -10.238 | 1.00 | 0.00 |
| ATOM | 1184 | HO1 | VAL | 72 | 1.944 | -2.028 | -1.895 | 1.00 | 0.00 |
| ATOM | 1185 | HO2 | VAL | 72 | 7.419 | -2.028 | -1.895 | 1.00 | 0.00 |
| ATOM | 1186 | CD | VAL | 72 | 8.261 | -0.980 | -9.305 | 1.00 | 0.00 |
| ATOM | 1187 | CG | VAL | 72 | 7.728 | -0.975 | -9.615 | 1.00 | 0.00 |
| ATOM | 1188 | CG1 | VAL | 72 | 6.339 | -0.915 | -10.258 | 1.00 | 0.00 |
| ATOM | 1189 | CG2 | VAL | 72 | 5.985 | -0.915 | -10.258 | 1.00 | 0.00 |
| ATOM | 1190 | CD | VAL | 72 | 6.224 | -0.005 | -10.258 | 1.00 | 0.00 |
| ATOM | 1191 | CD | VAL | 72 | 6.264 | -0.005 | -10.258 | 1.00 | 0.00 |
| ATOM | 1192 | CD | VAL | 72 | 6.264 | -0.005 | -10.258 | 1.00 | 0.00 |
| ATOM | 1193 | CD | VAL | 72 | 6.264 | -0.005 | -10.258 | 1.00 | 0.00 |
| ATOM | 1194 | CD | VAL | 72 | 6.264 | -0.005 | -10.258 | 1.00 | 0.00 |
| ATOM | 1195 | CD | VAL | 72 | 6.264 | -0.005 | -10.258 | 1.00 | 0.00 |
| ATOM | 1196 | CD | VAL | 72 | 6.264 | -0.005 | -10.258 | 1.00 | 0.00 |
| ATOM | 1197 | CD | VAL | 72 | 6.264 | -0.005 | -10.258 | 1.00 | 0.00 |
| ATOM | 1198 | CD | VAL | 72 | 6.264 | -0.005 | -10.258 | 1.00 | 0.00 |
| ATOM | 1199 | CD | VAL | 72 | 6.264 | -0.005 | -10.258 | 1.00 | 0.00 |
| ATOM | 1200 | CD | VAL | 72 | 6.264 | -0.005 | -10.258 | 1.00 | 0.00 |
| ATOM | 1201 | CD | VAL | 72 | 6.264 | -0.005 | -10.258 | 1.00 | 0.00 |
| ATOM | 1202 | CD | VAL | 72 | 6.264 | -0.005 | -10.258 | 1.00 | 0.00 |
| ATOM | 1203 | CA | VAL | 72 | 6.264 | -0.005 | -10.258 | 1.00 | 0.00 |
| ATOM | 1204 | CB | VAL | 72 | 6.264 | -0.005 | -10.258 | 1.00 | 0.00 |
| ATOM | 1205 | CG | VAL | 72 | 6.264 | -0.005 | -10.258 | 1.00 | 0.00 |
| ATOM | 1206 | CD | VAL | 72 | 6.264 | -0.005 | -10.258 | 1.00 | 0.00 |
| ATOM | 1207 | CB | VAL | 72 | 6.264 | -0.005 | -10.258 | 1.00 | 0.00 |
| ATOM | 1208 | CG | VAL | 72 | 6.264 | -0.005 | -10.258 | 1.00 | 0.00 |
| ATOM | 1209 | CD | VAL | 72 | 6.264 | -0.005 | -10.258 | 1.00 | 0.00 |
| ATOM | 1210 | CB | VAL | 72 | 6.264 | -0.005 | -10.258 | 1.00 | 0.00 |
| ATOM | 1211 | CD | VAL | 72 | 6.264 | -0.005 | -10.258 | 1.00 | 0.00 |
| ATOM | 1212 | CB | VAL | 72 | 6.264 | -0.005 | -10.258 | 1.00 | 0.00 |
| ATOM | 1213 | CD | VAL | 72 | 6.264 | -0.005 | -10.258 | 1.00 | 0.00 |
| ATOM | 1214 | CB | VAL | 72 | 6.264 | -0.005 | -10.258 | 1.00 | 0.00 |
| ATOM | 1215 | CD | VAL | 72 | 6.264 | -0.005 | -10.258 | 1.00 | 0.00 |
| ATOM | 1216 | CB | VAL | 72 | 6.264 | -0.005 | -10.258 | 1.00 | 0.00 |
| ATOM | 1217 | CD | VAL | 72 | 6.264 | -0.005 | -10.258 | 1.00 | 0.00 |
| ATOM | 1218 | CB | VAL | 72 | 6.264 | -0.005 | -10.258 | 1.00 | 0.00 |
| ATOM | 1219 | CD | VAL | 72 | 6.264 | -0.005 | -10.258 | 1.00 | 0.00 |
| ATOM | 1220 | CB | VAL | 72 | 6.264 | -0.005 | -10.258 | 1.00 | 0.00 |
| ATOM | 1221 | CD | VAL | 72 | 6.264 | -0.005 | -10.258 | 1.00 | 0.00 |
| ATOM | 1222 | CB | VAL | 72 | 6.264 | -0.005 | -10.258 | 1.00 | 0.00 |
| ATOM | 1223 | CD | VAL | 72 | 6.264 | -0.005 | -10.258 | 1.00 | 0.00 |
| ATOM | 1224 | CB | VAL | 72 | 6.264 | -0.005 | -10.258 | 1.00 | 0.00 |
| ATOM | 1225 | CD | VAL | 72 | 6.264 | -0.005 | -10.258 | 1.00 | 0.00 |
| ATOM | 1226 | CB | VAL | 72 | 6.264 | -0.005 | -10.258 | 1.00 | 0.00 |
| ATOM | 1227 | CD | VAL | 72 | 6.264 | -0.005 | -10.258 | 1.00 | 0.00 |
| ATOM | 1228 | CB | VAL | 72 | | | | | |

REPLACEMENT SHEET

| | | | | | | | | | |
|------|------|------|-----|----|---------|---------|--------|------|--------|
| ATOM | 1383 | C02 | THR | 83 | -4.464 | -7.286 | 5.619 | 1.00 | 0.00 |
| ATOM | 1384 | H02 | THR | 83 | -3.654 | -7.40 | 6.333 | 1.00 | 0.00 |
| ATOM | 1385 | H022 | THR | 83 | -4.384 | -8.25 | 5.389 | 1.00 | 0.00 |
| ATOM | 1386 | H023 | THR | 83 | -5.228 | 6.656 | 6.048 | 1.00 | 0.00 |
| ATOM | 1387 | C | THR | 83 | -2.778 | 6.017 | 3.711 | 1.00 | 0.00 |
| ATOM | 1388 | O | THR | 83 | -6.221 | 4.033 | 4.033 | 1.00 | 0.00 |
| ATOM | 1389 | N | ASN | 84 | -6.333 | 4.690 | 3.756 | 1.00 | 0.00 |
| ATOM | 1390 | H | ASN | 84 | -5.550 | 4.376 | 4.376 | 1.00 | 0.00 |
| ATOM | 1391 | CA | ASN | 84 | -7.533 | 3.987 | 4.190 | 1.00 | 0.00 |
| ATOM | 1392 | HA | ASN | 84 | -7.822 | 4.381 | 5.183 | 1.00 | 0.00 |
| ATOM | 1393 | CB | ASN | 84 | -7.250 | 2.491 | 4.321 | 1.00 | 0.00 |
| ATOM | 1394 | HBL | ASN | 84 | -6.457 | 2.342 | 5.039 | 1.00 | 0.00 |
| ATOM | 1395 | B02 | ASN | 84 | -6.939 | 2.087 | 3.362 | 1.00 | 0.00 |
| ATOM | 1396 | CG | ASN | 84 | -6.464 | 1.707 | 4.778 | 1.00 | 0.00 |
| ATOM | 1397 | O01 | ASN | 84 | -9.459 | 2.282 | 5.218 | 1.00 | 0.00 |
| ATOM | 1398 | NDC | ASN | 84 | -8.388 | 0.385 | 4.672 | 1.00 | 0.00 |
| ATOM | 1399 | H021 | ASN | 84 | -7.354 | -0.004 | 4.112 | 1.00 | 0.00 |
| ATOM | 1400 | H022 | ASN | 84 | -9.158 | -0.447 | 4.960 | 1.00 | 0.00 |
| ATOM | 1401 | C | ASN | 84 | -8.670 | -2.122 | -3.201 | 1.00 | 0.00 |
| ATOM | 1402 | O | ASN | 84 | -9.636 | -4.879 | -3.554 | 1.00 | 0.00 |
| ATOM | 1403 | N | CYS | 85 | -8.520 | -2.023 | 1.000 | 1.00 | 0.00 |
| ATOM | 1404 | H | CYS | 85 | -7.708 | -1.142 | -1.812 | 1.00 | 0.00 |
| ATOM | 1405 | CA | CYS | 85 | -7.526 | -0.908 | -0.961 | 1.00 | 0.00 |
| ATOM | 1406 | O | CYS | 85 | -10.414 | -0.280 | 1.276 | 1.00 | 0.00 |
| ATOM | 1407 | G01 | CYS | 85 | -9.228 | -0.005 | 4.134 | 1.00 | 0.00 |
| ATOM | 1408 | HE1 | CYS | 85 | -9.789 | -0.322 | 1.109 | 1.00 | 0.00 |
| ATOM | 1409 | HE2 | CYS | 85 | -8.132 | -1.724 | 0.595 | 1.00 | 0.00 |
| ATOM | 1410 | M | CYS | 85 | -9.935 | -0.585 | 1.501 | 1.00 | 0.00 |
| ATOM | 1411 | MG | CYS | 85 | -9.931 | -0.652 | 1.100 | 1.00 | 0.00 |
| ATOM | 1412 | C | CYS | 85 | -10.395 | -0.578 | 0.598 | 1.00 | 0.00 |
| ATOM | 1413 | O | CYS | 85 | -10.995 | -0.563 | 0.598 | 1.00 | 0.00 |
| ATOM | 1414 | N | LYS | 86 | -1.593 | -0.999 | 1.200 | 1.00 | 0.00 |
| ATOM | 1415 | H | LYS | 86 | -8.822 | -5.82 | -1.288 | 1.00 | 0.00 |
| ATOM | 1416 | CA | LYS | 86 | -9.103 | -3.005 | 1.334 | 1.00 | 0.00 |
| ATOM | 1417 | HA | LYS | 86 | -9.725 | -5.76 | -0.840 | 1.00 | 0.00 |
| ATOM | 1418 | CB | LYS | 86 | -7.758 | -8.299 | -0.629 | 1.00 | 0.00 |
| ATOM | 1419 | HBL | LYS | 86 | -7.355 | -7.988 | -0.630 | 1.00 | 0.00 |
| ATOM | 1420 | H02 | LYS | 86 | -7.078 | -7.990 | -0.630 | 1.00 | 0.00 |
| ATOM | 1421 | CG | LYS | 86 | -7.653 | -9.807 | -0.632 | 1.00 | 0.00 |
| ATOM | 1422 | G01 | LYS | 86 | -8.858 | -10.091 | -0.561 | 1.00 | 0.00 |
| ATOM | 1423 | HE2 | LYS | 86 | -7.623 | -10.178 | -0.566 | 1.00 | 0.00 |
| ATOM | 1424 | CD | LYS | 86 | -6.882 | -10.42 | -1.656 | 1.00 | 0.00 |
| ATOM | 1425 | HD0 | LYS | 86 | -6.363 | -11.427 | -2.334 | 1.00 | 0.00 |
| ATOM | 1426 | H02 | LYS | 86 | -5.960 | -9.633 | -2.147 | 1.00 | 0.00 |
| ATOM | 1427 | CE | LYS | 86 | -5.359 | -11.376 | -0.930 | 1.00 | 0.00 |
| ATOM | 1428 | HE1 | LYS | 86 | -5.744 | -11.108 | -0.690 | 1.00 | 0.00 |
| ATOM | 1429 | HE2 | LYS | 86 | -4.915 | -11.221 | -1.447 | 1.00 | 0.00 |
| ATOM | 1430 | NZ | LYS | 86 | -6.277 | -12.718 | -0.922 | 1.00 | 0.00 |
| ATOM | 1431 | H21 | LYS | 86 | -6.207 | -13.125 | -0.441 | 1.00 | 0.00 |
| ATOM | 1432 | H22 | LYS | 86 | -7.360 | -13.025 | -1.249 | 1.00 | 0.00 |
| ATOM | 1433 | C02 | LYS | 86 | -9.005 | -8.175 | -2.060 | 1.00 | 0.00 |
| ATOM | 1434 | C | LYS | 86 | -9.669 | -6.662 | -5.462 | 1.00 | 0.00 |
| ATOM | 1435 | O | LYS | 86 | -10.579 | -9.266 | -3.943 | 1.00 | 0.00 |
| ATOM | 1436 | N | LGL | 87 | -9.188 | -7.618 | -3.220 | 1.00 | 0.00 |
| ATOM | 1437 | H | GLU | 87 | -8.883 | -6.866 | -3.559 | 1.00 | 0.00 |
| ATOM | 1438 | CA | GLU | 87 | -10.101 | -8.013 | -4.474 | 1.00 | 0.00 |
| ATOM | 1439 | HA | GLU | 87 | -10.483 | -8.455 | -4.100 | 1.00 | 0.00 |
| ATOM | 1440 | CB | GLU | 87 | -9.384 | -7.684 | -4.665 | 1.00 | 0.00 |
| ATOM | 1441 | HE1 | GLU | 87 | -13.392 | -9.172 | -5.582 | 1.00 | 0.00 |
| ATOM | 1442 | HE2 | GLU | 87 | -9.663 | -6.362 | -5.462 | 1.00 | 0.00 |
| ATOM | 1443 | CG | GLU | 87 | -9.084 | -5.570 | -5.963 | 1.00 | 0.00 |
| ATOM | 1444 | HD0 | GLU | 87 | -9.284 | -7.126 | -5.909 | 1.00 | 0.00 |
| ATOM | 1445 | HD1 | GLU | 87 | -7.359 | -6.444 | -5.904 | 1.00 | 0.00 |
| ATOM | 1446 | OD0 | GLU | 87 | -8.460 | -9.007 | -6.907 | 1.00 | 0.00 |
| ATOM | 1447 | OD1 | GLU | 87 | -9.007 | -9.593 | -6.907 | 1.00 | 0.00 |
| ATOM | 1448 | OE2 | GLU | 87 | -7.316 | -10.131 | -6.907 | 1.00 | 0.00 |
| ATOM | 1449 | CGU | GLU | 87 | -11.539 | -7.621 | -6.645 | 1.00 | 0.00 |
| ATOM | 1450 | O | GLU | 87 | -12.422 | -8.997 | -6.610 | 1.00 | 0.00 |
| ATOM | 1451 | N | TYR | 88 | -11.165 | -6.338 | -4.387 | 1.00 | 0.00 |
| ATOM | 1452 | H | TYR | 88 | -11.023 | -5.763 | -4.109 | 1.00 | 0.00 |
| ATOM | 1453 | CA | TYR | 88 | -11.100 | -5.474 | -4.536 | 1.00 | 0.00 |
| ATOM | 1454 | HA | TYR | 88 | -11.320 | -5.026 | -4.549 | 1.00 | 0.00 |
| ATOM | 1455 | CB | TYR | 88 | -11.000 | -4.234 | -4.639 | 1.00 | 0.00 |
| ATOM | 1456 | HE1 | TYR | 88 | -12.032 | -5.040 | -4.000 | 1.00 | 0.00 |
| ATOM | 1457 | HE2 | TYR | 88 | -13.100 | -5.653 | -5.000 | 1.00 | 0.00 |
| ATOM | 1458 | CG | TYR | 88 | -14.055 | -6.162 | -5.527 | 1.00 | 0.00 |
| ATOM | 1459 | CD1 | TYR | 88 | -15.165 | -2.981 | -4.982 | 1.00 | 0.00 |
| ATOM | 1460 | HDI | TYR | 88 | -15.273 | -2.942 | -3.308 | 1.00 | 0.00 |
| ATOM | 1461 | CD2 | TYR | 88 | -13.935 | -6.561 | -6.911 | 1.00 | 0.00 |
| ATOM | 1462 | H02 | TYR | 88 | -13.076 | -6.144 | -7.350 | 1.00 | 0.00 |
| ATOM | 1463 | HE1 | TYR | 88 | -14.130 | -5.790 | -6.000 | 1.00 | 0.00 |
| ATOM | 1464 | HE2 | TYR | 88 | -14.987 | -5.347 | -5.100 | 1.00 | 0.00 |
| ATOM | 1465 | C02 | TYR | 88 | -14.999 | -5.987 | -5.400 | 1.00 | 0.00 |
| ATOM | 1466 | H022 | TYR | 88 | -14.785 | -6.800 | -6.000 | 1.00 | 0.00 |
| ATOM | 1467 | CZ | TYR | 88 | -15.990 | -2.463 | -7.161 | 1.00 | 0.00 |
| ATOM | 1468 | OH | TYR | 88 | -16.947 | -1.993 | -7.569 | 1.00 | 0.00 |
| ATOM | 1469 | CD | TYR | 88 | -17.473 | -2.84 | -6.378 | 1.00 | 0.00 |
| ATOM | 1470 | C | TYR | 88 | -14.010 | -6.637 | -3.368 | 1.00 | 0.00 |
| ATOM | 1471 | O | TYR | 88 | -14.955 | -5.265 | -2.691 | 1.00 | 0.00 |
| ATOM | 1472 | N | TYR | 88 | -14.187 | -4.931 | -3.150 | 1.00 | 0.00 |
| ATOM | 1473 | HN | ASN | 89 | -13.337 | -3.777 | -1.000 | 0.00 | 0.00 |
| ATOM | 1474 | AS | ASN | 89 | -13.338 | -3.777 | -1.000 | 0.00 | 0.00 |
| ATOM | 1475 | CB | ASN | 89 | -13.338 | -3.776 | -1.000 | 0.00 | 0.00 |
| ATOM | 1476 | CG | ASN | 89 | -13.338 | -3.776 | -1.000 | 0.00 | 0.00 |
| ATOM | 1477 | HB1 | ASN | 89 | -13.338 | -3.776 | -1.000 | 0.00 | 0.00 |
| ATOM | 1478 | HB2 | ASN | 89 | -13.338 | -3.776 | -1.000 | 0.00 | 0.00 |
| ATOM | 1479 | CG | ASN | 89 | -13.338 | -3.776 | -1.000 | 0.00 | 0.00 |
| ATOM | 1480 | CD | ASN | 89 | -13.338 | -3.776 | -1.000 | 0.00 | 0.00 |
| ATOM | 1481 | ND2 | ASN | 89 | -13.338 | -3.776 | -1.000 | 0.00 | 0.00 |
| ATOM | 1482 | OD2 | ASN | 89 | -13.338 | -3.776 | -1.000 | 0.00 | 0.00 |
| ATOM | 1483 | CB | ASN | 89 | -13.338 | -3.776 | -1.000 | 0.00 | 0.00 |
| ATOM | 1484 | CD2 | ASN | 89 | -13.338 | -3.776 | -1.000 | 0.00 | 0.00 |
| ATOM | 1485 | OD2 | ASN | 89 | -13.338 | -3.776 | -1.000 | 0.00 | 0.00 |
| ATOM | 1486 | CG | ASN | 89 | -13.338 | -3.776 | -1.000 | 0.00 | 0.00 |
| ATOM | 1487 | CD | ASN | 89 | -13.338 | -3.776 | -1.000 | 0.00 | 0.00 |
| ATOM | 1488 | OD | ASN | 89 | -13.338 | -3.776 | -1.000 | 0.00 | 0.00 |
| ATOM | 1489 | CB | ASN | 89 | -13.338 | -3.776 | -1.000 | 0.00 | 0.00 |
| ATOM | 1490 | CD2 | ASN | 89 | -13.338 | -3.776 | -1.000 | 0.00 | 0.00 |
| ATOM | 1491 | OD2 | ASN | 89 | -13.338 | -3.776 | -1.000 | 0.00 | 0.00 |
| ATOM | 1492 | CG | ASN | 89 | -13.338 | -3.776 | -1.000 | 0.00 | 0.00 |
| ATOM | 1493 | CD | ASN | 89 | -13.338 | -3.776 | -1.000 | 0.00 | 0.00 |
| ATOM | 1494 | OD | ASN | 89 | -13.338 | -3.776 | -1.000 | 0.00 | 0.00 |
| ATOM | 1495 | CB | ASN | 89 | -13.338 | -3.776 | -1.000 | 0.00 | 0.00 |
| ATOM | 1496 | CD2 | ASN | 89 | -13.338 | -3.776 | -1.000 | 0.00 | 0.00 |
| ATOM | 1497 | OD2 | ASN | 89 | -13.338 | -3.776 | -1.000 | 0.00 | 0.00 |
| ATOM | 1498 | CG | ASN | 89 | -13.338 | -3.776 | -1.000 | 0.00 | 0.00 |
| ATOM | 1499 | CD | ASN | 89 | -13.338 | -3.776 | -1.000 | 0.00 | 0.00 |
| ATOM | 1500 | OD | ASN | 89 | -13.338 | -3.776 | -1.000 | 0.00 | 0.00 |
| ATOM | 1501 | CB | ASN | 89 | -13.338 | -3.776 | -1.000 | 0.00 | 0.00 |
| ATOM | 1502 | CD2 | ASN | 89 | -13.338 | -3.776 | -1.000 | 0.00 | 0.00 |
| ATOM | 1503 | OD2 | ASN | 89 | -13.338 | -3.776 | -1.000 | 0.00 | 0.00 |
| ATOM | 1504 | CG | ASN | 89 | -13.338 | -3.776 | -1.000 | 0.00 | 0.00 |
| ATOM | 1505 | CD | ASN | 89 | -13.338 | -3.776 | -1.000 | 0.00 | 0.00 |
| ATOM | 1506 | OD | ASN | 89 | -13.338 | -3.776 | -1.000 | 0.00 | 0.00 |
| ATOM | 1507 | CB | ASN | 89 | -13.338 | -3.776 | -1.000 | 0.00 | 0.00 |
| ATOM | 1508 | CD2 | ASN | 89 | -13.338 | -3.776 | -1.000 | 0.00 | 0.00 |
| ATOM | 1509 | OD2 | ASN | 89 | -13.338 | -3.776 | -1.000 | 0.00 | 0.00</ |

REPLACEMENT SHEET

| | | | | | | | | | |
|------|------|------|-----|-----|--------|--------|--------|------|------|
| ATOM | 1655 | HDL2 | ILE | 101 | -6.07 | 5.842 | 11.709 | 1.00 | 0.00 |
| ATOM | 1666 | HDL3 | ILE | 101 | -7.84 | 5.966 | 10.554 | 1.00 | 0.00 |
| ATOM | 1667 | C | ILE | 101 | -2.51 | 6.457 | 8.226 | 1.00 | 0.00 |
| ATOM | 1668 | O | ILE | 101 | -1.35 | 6.607 | 8.312 | 1.00 | 0.00 |
| ATOM | 1669 | N | ILE | 102 | -2.876 | 5.943 | 9.500 | 1.00 | 0.00 |
| ATOM | 1670 | HN | ILE | 102 | -3.829 | 5.117 | 7.527 | 1.00 | 0.00 |
| ATOM | 1671 | CA | ILE | 102 | -1.886 | 4.575 | 6.972 | 1.00 | 0.00 |
| ATOM | 1672 | CB | ILE | 102 | -1.350 | 3.953 | 7.763 | 1.00 | 0.00 |
| ATOM | 1673 | CH | ILE | 102 | -2.569 | 3.162 | 6.012 | 1.00 | 0.00 |
| ATOM | 1674 | HE1 | ILE | 102 | -1.630 | 3.443 | 6.283 | 1.00 | 0.00 |
| ATOM | 1675 | HE2 | ILE | 102 | -2.408 | 3.700 | 6.933 | 1.00 | 0.00 |
| ATOM | 1676 | HE3 | ILE | 102 | -2.083 | 3.971 | 5.260 | 1.00 | 0.00 |
| ATOM | 1677 | HG | ILE | 102 | -2.423 | 1.982 | 4.200 | 1.00 | 0.00 |
| ATOM | 1678 | HEO | ILE | 102 | -2.676 | 1.864 | 5.753 | 1.00 | 0.00 |
| ATOM | 1679 | MET1 | ILE | 102 | -1.493 | 1.195 | 3.156 | 1.00 | 0.00 |
| ATOM | 1680 | MET2 | ILE | 102 | -2.958 | 0.338 | 3.732 | 1.00 | 0.00 |
| ATOM | 1681 | MET3 | ILE | 102 | -0.549 | 1.288 | 6.812 | 1.00 | 0.00 |
| ATOM | 1682 | MET4 | ILE | 102 | -0.559 | 2.499 | 6.220 | 1.00 | 0.00 |
| ATOM | 1683 | MET5 | ILE | 102 | -0.447 | 2.978 | 5.749 | 1.00 | 0.00 |
| ATOM | 1684 | MET6 | ILE | 102 | -0.524 | 1.907 | 7.213 | 1.00 | 0.00 |
| ATOM | 1685 | MET7 | ILE | 102 | -0.522 | 1.556 | 6.565 | 1.00 | 0.00 |
| ATOM | 1686 | MET8 | ILE | 102 | -0.697 | 1.117 | 1.179 | 1.00 | 0.00 |
| ATOM | 1687 | O | ILE | 102 | -0.303 | 4.984 | 6.965 | 1.00 | 0.00 |
| ATOM | 1688 | N | ILE | 103 | -1.144 | 6.366 | 5.433 | 1.00 | 0.00 |
| ATOM | 1689 | HN | ILE | 103 | -2.171 | 6.439 | 5.498 | 1.00 | 0.00 |
| ATOM | 1690 | CA | ILE | 103 | -0.581 | 7.132 | 6.624 | 1.00 | 0.00 |
| ATOM | 1691 | CB | ILE | 103 | -0.056 | 6.512 | 3.960 | 1.00 | 0.00 |
| ATOM | 1692 | CG | ILE | 103 | -1.446 | 8.146 | 3.857 | 1.00 | 0.00 |
| ATOM | 1693 | HR1 | ILE | 103 | -0.912 | 8.800 | 4.572 | 1.00 | 0.00 |
| ATOM | 1694 | HR2 | ILE | 103 | -2.220 | 7.611 | 3.120 | 1.00 | 0.00 |
| ATOM | 1695 | CGU | ILE | 103 | -0.670 | 8.991 | 2.860 | 1.00 | 0.00 |
| ATOM | 1696 | HGU | ILE | 103 | -1.083 | 8.832 | 1.874 | 1.00 | 0.00 |
| ATOM | 1697 | RGU | ILE | 103 | -0.364 | 8.891 | 2.871 | 1.00 | 0.00 |
| ATOM | 1698 | GDU | ILE | 103 | -0.734 | 10.042 | 3.347 | 1.00 | 0.00 |
| ATOM | 1699 | QEL | ILE | 103 | -0.556 | 10.596 | 3.342 | 1.00 | 0.00 |
| ATOM | 1700 | QER | ILE | 103 | -0.337 | 11.108 | 3.264 | 1.00 | 0.00 |
| ATOM | 1701 | C | GLU | 103 | -0.439 | 7.955 | 4.578 | 1.00 | 0.00 |
| ATOM | 1702 | O | GLU | 103 | -1.644 | 7.658 | 3.534 | 1.00 | 0.00 |
| ATOM | 1703 | N | GLU | 103 | -0.552 | 6.405 | 4.000 | 1.00 | 0.00 |
| ATOM | 1704 | HN | GLU | 104 | -0.782 | 6.480 | 1.000 | 1.00 | 0.00 |
| ATOM | 1705 | CA | GLU | 104 | -0.221 | 9.117 | 7.306 | 1.00 | 0.00 |
| ATOM | 1706 | CD | GLU | 104 | -1.329 | 10.172 | 6.775 | 1.00 | 0.00 |
| ATOM | 1707 | OD1 | GLU | 104 | -0.003 | 10.040 | 6.248 | 1.00 | 0.00 |
| ATOM | 1708 | OD2 | GLU | 104 | -0.949 | 9.949 | 8.492 | 1.00 | 0.00 |
| ATOM | 1709 | HB2 | LYS | 104 | -0.530 | 10.024 | 9.315 | 1.00 | 0.00 |
| ATOM | 1710 | CG | LYS | 104 | -2.078 | 11.156 | 9.125 | 1.00 | 0.00 |
| ATOM | 1711 | HG | LYS | 104 | -0.635 | 12.128 | 2.601 | 1.00 | 0.00 |
| ATOM | 1712 | HC2 | LYS | 104 | -1.026 | 11.920 | 9.820 | 1.00 | 0.00 |
| ATOM | 1713 | HC1 | LYS | 104 | -2.239 | 14.433 | 6.661 | 1.00 | 0.00 |
| ATOM | 1714 | HD1 | LYS | 104 | -0.782 | 10.786 | 7.088 | 1.00 | 0.00 |
| ATOM | 1715 | HD2 | LYS | 104 | -0.293 | 10.024 | 9.316 | 1.00 | 0.00 |
| ATOM | 1716 | HD3 | LYS | 104 | -0.960 | 12.322 | 6.447 | 1.00 | 0.00 |
| ATOM | 1717 | HE1 | LYS | 104 | -2.073 | 12.989 | 6.695 | 1.00 | 0.00 |
| ATOM | 1718 | HE2 | LYS | 104 | -2.601 | 12.984 | 5.954 | 1.00 | 0.00 |
| ATOM | 1719 | HE3 | LYS | 104 | -1.877 | 14.053 | 6.791 | 1.00 | 0.00 |
| ATOM | 1720 | EL1 | LYS | 104 | -2.226 | 11.920 | 9.820 | 1.00 | 0.00 |
| ATOM | 1721 | EL2 | LYS | 104 | -2.239 | 14.433 | 6.661 | 1.00 | 0.00 |
| ATOM | 1722 | EL3 | LYS | 104 | -0.782 | 10.786 | 7.088 | 1.00 | 0.00 |
| ATOM | 1723 | CD | LYS | 104 | -0.293 | 10.024 | 9.316 | 1.00 | 0.00 |
| ATOM | 1724 | CG | LYS | 104 | -0.960 | 12.322 | 6.447 | 1.00 | 0.00 |
| ATOM | 1725 | HN | LYS | 104 | -2.073 | 12.984 | 5.954 | 1.00 | 0.00 |
| ATOM | 1726 | C | LYS | 104 | -2.601 | 12.984 | 5.954 | 1.00 | 0.00 |
| ATOM | 1727 | CA | LYS | 104 | -2.226 | 11.920 | 9.820 | 1.00 | 0.00 |
| ATOM | 1728 | CB | LYS | 104 | -2.239 | 14.433 | 6.661 | 1.00 | 0.00 |
| ATOM | 1729 | CH | LYS | 104 | -0.782 | 10.786 | 7.088 | 1.00 | 0.00 |
| ATOM | 1730 | CD1 | LYS | 104 | -0.293 | 10.024 | 9.316 | 1.00 | 0.00 |
| ATOM | 1731 | CB2 | LYS | 105 | -0.540 | 9.077 | 8.811 | 1.00 | 0.00 |
| ATOM | 1732 | CG | LYS | 105 | -1.411 | 9.565 | 11.031 | 1.00 | 0.00 |
| ATOM | 1733 | COL | LYS | 105 | -2.955 | 10.294 | 11.524 | 1.00 | 0.00 |
| ATOM | 1734 | HDL1 | LYS | 105 | -0.523 | 9.687 | 10.853 | 1.00 | 0.00 |
| ATOM | 1735 | COL2 | LYS | 105 | -0.083 | 9.687 | 10.853 | 1.00 | 0.00 |
| ATOM | 1736 | CD2 | LYS | 105 | -2.177 | 11.874 | 11.874 | 1.00 | 0.00 |
| ATOM | 1737 | CEL | PHR | 105 | -0.491 | 8.877 | 11.478 | 1.00 | 0.00 |
| ATOM | 1738 | HE1 | PHR | 105 | -0.296 | 9.190 | 12.285 | 1.00 | 0.00 |
| ATOM | 1739 | CER | PHR | 105 | -2.051 | 4.783 | 13.241 | 1.00 | 0.00 |
| ATOM | 1740 | HER2 | PHR | 105 | -2.665 | 4.786 | 13.911 | 1.00 | 0.00 |
| ATOM | 1741 | CZ | PHR | 105 | -1.172 | 13.750 | 1.000 | 1.00 | 0.00 |
| ATOM | 1742 | HZ | PHR | 105 | -0.079 | 14.818 | 8.818 | 1.00 | 0.00 |
| ATOM | 1743 | C | PHR | 105 | -2.379 | 5.655 | 7.785 | 1.00 | 0.00 |
| ATOM | 1744 | O | PHR | 105 | -4.911 | 5.877 | 7.808 | 1.00 | 0.00 |
| ATOM | 1745 | N | PHR | 106 | -2.702 | 4.870 | 6.882 | 1.00 | 0.00 |
| ATOM | 1746 | HN | PHR | 106 | -1.732 | 6.922 | 1.000 | 0.00 | 0.00 |
| ATOM | 1747 | CH | PHR | 106 | -4.770 | 4.199 | 5.841 | 1.00 | 0.00 |
| ATOM | 1748 | CB | PHR | 106 | -4.078 | 3.441 | 6.316 | 1.00 | 0.00 |
| ATOM | 1749 | CG | PHR | 106 | -2.532 | 2.886 | 8.919 | 1.00 | 0.00 |
| ATOM | 1750 | HL1 | PHR | 106 | -1.881 | 2.844 | 5.666 | 1.00 | 0.00 |
| ATOM | 1751 | HL2 | PHR | 106 | -1.937 | 2.881 | 5.351 | 1.00 | 0.00 |
| ATOM | 1752 | CG | PHR | 106 | -2.524 | 2.755 | 7.777 | 1.00 | 0.00 |
| ATOM | 1753 | CD1 | PHR | 106 | -1.596 | 1.077 | 1.077 | 1.00 | 0.00 |
| ATOM | 1754 | CD2 | PHR | 106 | -1.928 | 1.077 | 1.077 | 1.00 | 0.00 |
| ATOM | 1755 | CE1 | PHR | 106 | -2.063 | 1.076 | 1.076 | 1.00 | 0.00 |
| ATOM | 1756 | CE2 | PHR | 106 | -1.737 | 1.076 | 1.076 | 1.00 | 0.00 |
| ATOM | 1757 | CH1 | PHR | 106 | -1.737 | 1.076 | 1.076 | 1.00 | 0.00 |
| ATOM | 1758 | HE1 | PHR | 106 | -0.022 | 3.776 | 3.776 | 1.00 | 0.00 |
| ATOM | 1759 | CD2 | PHR | 106 | -1.737 | 1.076 | 1.076 | 1.00 | 0.00 |
| ATOM | 1760 | CD3 | PHR | 106 | -1.737 | 1.076 | 1.076 | 1.00 | 0.00 |
| ATOM | 1761 | CG2 | PHR | 106 | -1.737 | 1.076 | 1.076 | 1.00 | 0.00 |
| ATOM | 1762 | CG3 | PHR | 106 | -1.737 | 1.076 | 1.076 | 1.00 | 0.00 |
| ATOM | 1763 | CG4 | PHR | 106 | -1.737 | 1.076 | 1.076 | 1.00 | 0.00 |
| ATOM | 1764 | CG5 | PHR | 106 | -1.737 | 1.076 | 1.076 | 1.00 | 0.00 |
| ATOM | 1765 | CG6 | PHR | 106 | -1.737 | 1.076 | 1.076 | 1.00 | 0.00 |
| ATOM | 1766 | CG7 | PHR | 106 | -1.737 | 1.076 | 1.076 | 1.00 | 0.00 |
| ATOM | 1767 | CG8 | PHR | 106 | -1.737 | 1.076 | 1.076 | 1.00 | 0.00 |
| ATOM | 1768 | CG9 | PHR | 106 | -1.737 | 1.076 | 1.076 | 1.00 | 0.00 |
| ATOM | 1769 | CG10 | PHR | 106 | -1.737 | 1.076 | 1.076 | 1.00 | 0.00 |
| ATOM | 1770 | CG11 | PHR | 106 | -1.737 | 1.076 | 1.076 | 1.00 | 0.00 |
| ATOM | 1771 | CG12 | PHR | 106 | -1.737 | 1.076 | 1.076 | 1.00 | 0.00 |
| ATOM | 1772 | CG13 | PHR | 106 | -1.737 | 1.076 | 1.076 | 1.00 | 0.00 |
| ATOM | 1773 | CG14 | PHR | 106 | -1.737 | 1.076 | 1.076 | 1.00 | 0.00 |
| ATOM | 1774 | CG15 | PHR | 106 | -1.737 | 1.076 | 1.076 | 1.00 | 0.00 |
| ATOM | 1775 | CG16 | PHR | 106 | -1.737 | 1.076 | 1.076 | 1.00 | 0.00 |
| ATOM | 1776 | CG17 | PHR | 106 | -1.737 | 1.076 | 1.076 | 1.00 | 0.00 |
| ATOM | 1777 | CG18 | PHR | 106 | -1.737 | 1.076 | 1.076 | 1.00 | 0.00 |
| ATOM | 1778 | CG19 | PHR | 106 | -1.737 | 1.076 | 1.076 | 1.00 | 0.00 |
| ATOM | 1779 | CG20 | PHR | 106 | -1.737 | 1.076 | 1.076 | 1.00 | 0.00 |
| ATOM | 1780 | CG21 | PHR | 106 | -1.737 | 1.076 | 1.076 | 1.00 | 0.00 |
| ATOM | 1781 | CG22 | PHR | 106 | -1.737 | 1.076 | 1.076 | 1.00 | 0.00 |
| ATOM | 1782 | CG23 | PHR | 106 | -1.737 | 1.076 | 1.076 | 1.00 | 0.00 |
| ATOM | 1783 | CG24 | PHR | 106 | -1.737 | 1.076 | 1.076 | 1.00 | 0.00 |
| ATOM | 1784 | CG25 | PHR | 106 | -1.737 | 1.076 | 1.076 | 1.00 | 0.00 |
| ATOM | 1785 | CG26 | PHR | 106 | -1.737 | 1.076 | 1.076 | 1.00 | 0.00 |
| ATOM | 1786 | CG27 | PHR | 106 | -1.737 | 1.076 | 1.076 | 1.00 | 0.00 |
| ATOM | 1787 | CG28 | PHR | 106 | -1.737 | 1.076 | 1.076 | 1.00 | 0.00 |
| ATOM | 1788 | CG29 | PHR | 106 | -1.737 | 1.076 | 1.076 | 1.00 | 0.00 |
| ATOM | 1789 | CG30 | PHR | 106 | -1.7 | | | | |

REPLACEMENT SHEET

| | | | | | | | | | |
|------|------|------|-----|-----|--------|--------|--------|------|------|
| ATOM | 1947 | H2 | LVS | 119 | 4.432 | 9.001 | -5.028 | 1.00 | 0.00 |
| ATOM | 1948 | C2 | LVS | 119 | 3.921 | 10.506 | 5.527 | 1.00 | 0.00 |
| ATOM | 1949 | HC | LVS | 119 | 3.171 | 10.446 | 6.522 | 1.00 | 0.00 |
| ATOM | 1950 | HC | LVS | 119 | 3.077 | 11.595 | 6.522 | 1.00 | 0.00 |
| ATOM | 1951 | CD | LVS | 119 | 1.642 | 10.689 | 5.053 | 1.00 | 0.00 |
| ATOM | 1952 | HD | LVS | 118 | 1.422 | 9.100 | 5.449 | 1.00 | 0.00 |
| ATOM | 1953 | HD | LVS | 118 | 1.637 | 10.644 | 3.974 | 1.00 | 0.00 |
| ATOM | 1954 | CG | LVS | 118 | 0.569 | 11.055 | -5.518 | 1.00 | 0.00 |
| ATOM | 1955 | HE1 | LVS | 118 | -0.425 | 11.347 | -4.666 | 1.00 | 0.00 |
| ATOM | 1956 | HE2 | LVS | 118 | 1.048 | 11.922 | -5.942 | 1.00 | 0.00 |
| ATOM | 1957 | N2 | LVS | 118 | -0.324 | 10.443 | -6.543 | 1.00 | 0.00 |
| ATOM | 1958 | HE21 | LVS | 118 | -0.734 | 9.558 | -6.180 | 1.00 | 0.00 |
| ATOM | 1959 | HE22 | LVS | 119 | 0.214 | 10.223 | -7.498 | 1.00 | 0.00 |
| ATOM | 1960 | HE23 | LVS | 119 | -1.697 | 11.699 | -6.778 | 1.00 | 0.00 |
| ATOM | 1961 | C | LVS | 119 | 4.974 | 12.103 | -3.697 | 1.00 | 0.00 |
| ATOM | 1962 | OT1 | LVS | 119 | 4.769 | 13.177 | -4.291 | 1.00 | 0.00 |
| ATOM | 1963 | O12 | LVS | 119 | 4.901 | 11.986 | -2.445 | 1.00 | 0.00 |

END

Table 6

Atomic Structure Coordinates of the P/CAF Bromodomain/Acetyl-Histamine Complex

| | | | | | | | | | | | | | | | |
|--------|--------|------|------|----------|-----|----------|---|--------|--------|------|------|----------|-----|----------|---|
| 3.882 | -4.733 | 1.00 | 0.00 | BED ATOM | 151 | HDL ARG | 9 | 12.767 | -7.958 | 1.00 | 0.00 | BED ATOM | 65 | CIB MEC | 4 |
| 4.858 | -5.045 | 1.00 | 0.00 | BED ATOM | 152 | HDL ARG | 9 | 14.375 | -6.944 | 1.00 | 0.00 | BED ATOM | 67 | HBL MEC | 4 |
| 4.728 | -5.963 | 1.00 | 0.00 | BED ATOM | 153 | MBC ARG | 9 | 12.911 | -7.535 | 1.00 | 0.00 | BED ATOM | 73 | HBL MEC | 4 |
| 2.409 | -6.767 | 1.00 | 0.00 | BED ATOM | 154 | HB ARG | 9 | 14.490 | -7.006 | 1.00 | 0.00 | BED ATOM | 71 | SD CEC | 4 |
| 4.676 | -5.955 | 1.00 | 0.00 | BED ATOM | 155 | C2 ARG | 9 | 16.531 | -7.686 | 1.00 | 0.00 | BED ATOM | 74 | HEC MEC | 4 |
| 6.172 | -4.842 | 1.00 | 0.00 | BED ATOM | 156 | MH ARG | 9 | 16.443 | -7.576 | 1.00 | 0.00 | BED ATOM | 75 | HEC MEC | 4 |
| 4.006 | -4.006 | 1.00 | 0.00 | BED ATOM | 157 | HHL ARG | 9 | 17.289 | -7.049 | 1.00 | 0.00 | BED ATOM | 76 | MET CEC | 4 |
| 3.571 | -3.837 | 1.00 | 0.00 | BED ATOM | 158 | CD ARG | 9 | 17.929 | -7.851 | 1.00 | 0.00 | BED ATOM | 77 | MET CEC | 4 |
| 3.221 | -3.711 | 1.00 | 0.00 | BED ATOM | 159 | HA ARG | 9 | 11.997 | -6.126 | 1.00 | 0.00 | BED ATOM | 78 | N SER | 5 |
| 6.110 | -4.914 | 1.00 | 0.00 | BED ATOM | 160 | CH SER | 5 | 11.084 | -6.792 | 1.00 | 0.00 | BED ATOM | 79 | N SER | 5 |
| 11.194 | -7.759 | 1.00 | 0.00 | BED ATOM | 161 | HN SER | 5 | 11.194 | -7.559 | 1.00 | 0.00 | BED ATOM | 80 | HBL MEC | 4 |
| 9.939 | -6.125 | 1.00 | 0.00 | BED ATOM | 162 | HM SER | 5 | 9.939 | -6.677 | 1.00 | 0.00 | BED ATOM | 81 | SD CEC | 4 |
| 9.033 | -6.125 | 1.00 | 0.00 | BED ATOM | 163 | HB SER | 5 | 9.033 | -6.677 | 1.00 | 0.00 | BED ATOM | 82 | SD CEC | 4 |
| 7.448 | -7.111 | 1.00 | 0.00 | BED ATOM | 164 | HEI MEC | 4 | 7.448 | -7.111 | 1.00 | 0.00 | BED ATOM | 83 | HEI MEC | 4 |
| 5.960 | -6.786 | 1.00 | 0.00 | BED ATOM | 165 | HEC MEC | 4 | 5.960 | -7.000 | 1.00 | 0.00 | BED ATOM | 84 | HEC MEC | 4 |
| 17.289 | -7.049 | 1.00 | 0.00 | BED ATOM | 166 | HEZ MEC | 4 | 17.289 | -7.049 | 1.00 | 0.00 | BED ATOM | 85 | HEZ MEC | 4 |
| 5.560 | -5.851 | 1.00 | 0.00 | BED ATOM | 167 | HEZ SER | 5 | 5.560 | -6.000 | 1.00 | 0.00 | BED ATOM | 86 | HEZ SER | 5 |
| 11.906 | -6.000 | 1.00 | 0.00 | BED ATOM | 168 | HEZ SER | 5 | 11.906 | -6.000 | 1.00 | 0.00 | BED ATOM | 87 | HEZ SER | 5 |
| 6.114 | -6.601 | 1.00 | 0.00 | BED ATOM | 169 | HO SER | 5 | 6.114 | -6.601 | 1.00 | 0.00 | BED ATOM | 88 | HO SER | 5 |
| 8.624 | -6.423 | 1.00 | 0.00 | BED ATOM | 170 | HO LYS | 6 | 8.624 | -6.423 | 1.00 | 0.00 | BED ATOM | 89 | HO LYS | 6 |
| 10.189 | -4.819 | 1.00 | 0.00 | BED ATOM | 171 | HN SER | 5 | 10.189 | -4.819 | 1.00 | 0.00 | BED ATOM | 90 | HN SER | 5 |
| 9.833 | -3.999 | 1.00 | 0.00 | BED ATOM | 172 | HN LYS | 6 | 9.833 | -3.999 | 1.00 | 0.00 | BED ATOM | 91 | HN LYS | 6 |
| 11.227 | -5.665 | 1.00 | 0.00 | BED ATOM | 173 | CD LYS | 6 | 11.227 | -5.665 | 1.00 | 0.00 | BED ATOM | 92 | PA LYS | 6 |
| 8.565 | -4.410 | 1.00 | 0.00 | BED ATOM | 174 | PA LYS | 6 | 8.565 | -4.410 | 1.00 | 0.00 | BED ATOM | 93 | CT LYS | 6 |
| 9.801 | -5.172 | 1.00 | 0.00 | BED ATOM | 175 | HB1 LYS | 6 | 9.801 | -5.172 | 1.00 | 0.00 | BED ATOM | 94 | HB1 LYS | 6 |
| 9.056 | -5.056 | 1.00 | 0.00 | BED ATOM | 176 | HB2 LYS | 6 | 9.056 | -5.056 | 1.00 | 0.00 | BED ATOM | 95 | HB2 LYS | 6 |
| 8.624 | -4.148 | 1.00 | 0.00 | BED ATOM | 177 | CG LYS | 6 | 8.624 | -4.148 | 1.00 | 0.00 | BED ATOM | 96 | CG LYS | 6 |
| 10.189 | -4.677 | 1.00 | 0.00 | BED ATOM | 178 | HA LYS | 6 | 10.189 | -4.677 | 1.00 | 0.00 | BED ATOM | 97 | HA LYS | 6 |
| 11.227 | -5.665 | 1.00 | 0.00 | BED ATOM | 179 | HEI LYS | 6 | 11.227 | -5.665 | 1.00 | 0.00 | BED ATOM | 98 | HEI LYS | 6 |
| 10.299 | -5.665 | 1.00 | 0.00 | BED ATOM | 180 | HEC LYS | 6 | 10.299 | -5.665 | 1.00 | 0.00 | BED ATOM | 99 | HEC LYS | 6 |
| 8.879 | -5.000 | 1.00 | 0.00 | BED ATOM | 181 | HEZ LYS | 6 | 8.879 | -5.000 | 1.00 | 0.00 | BED ATOM | 100 | HEZ LYS | 6 |
| 11.546 | -6.155 | 1.00 | 0.00 | BED ATOM | 182 | CD SER | 5 | 11.546 | -6.155 | 1.00 | 0.00 | BED ATOM | 101 | CD SER | 5 |
| 10.024 | -5.150 | 1.00 | 0.00 | BED ATOM | 183 | HB1 SER | 5 | 10.024 | -5.150 | 1.00 | 0.00 | BED ATOM | 102 | HB1 SER | 5 |
| 13.203 | -6.166 | 1.00 | 0.00 | BED ATOM | 184 | HB2 SER | 5 | 13.203 | -6.166 | 1.00 | 0.00 | BED ATOM | 103 | HB2 SER | 5 |
| 13.089 | -4.949 | 1.00 | 0.00 | BED ATOM | 185 | HEI SER | 5 | 13.089 | -4.949 | 1.00 | 0.00 | BED ATOM | 104 | HEI SER | 5 |
| 13.953 | -3.991 | 1.00 | 0.00 | BED ATOM | 186 | HEC SER | 5 | 13.953 | -3.991 | 1.00 | 0.00 | BED ATOM | 105 | HEC SER | 5 |
| 13.645 | -2.302 | 1.00 | 0.00 | BED ATOM | 187 | HEZ SER | 5 | 13.645 | -2.302 | 1.00 | 0.00 | BED ATOM | 106 | HEZ SER | 5 |
| 13.576 | -2.070 | 1.00 | 0.00 | BED ATOM | 188 | CD SER | 5 | 13.576 | -2.070 | 1.00 | 0.00 | BED ATOM | 107 | CD SER | 5 |
| 14.632 | -2.189 | 1.00 | 0.00 | BED ATOM | 189 | HB1 SER | 5 | 14.632 | -2.189 | 1.00 | 0.00 | BED ATOM | 108 | HB1 SER | 5 |
| 9.720 | -2.613 | 1.00 | 0.00 | BED ATOM | 190 | HB2 SER | 5 | 9.720 | -2.613 | 1.00 | 0.00 | BED ATOM | 109 | HB2 SER | 5 |
| 9.022 | -2.026 | 1.00 | 0.00 | BED ATOM | 191 | HEI SER | 5 | 9.022 | -2.026 | 1.00 | 0.00 | BED ATOM | 110 | HEI SER | 5 |
| 7.474 | -2.334 | 1.00 | 0.00 | BED ATOM | 192 | HEC SER | 5 | 7.474 | -2.334 | 1.00 | 0.00 | BED ATOM | 111 | HEC SER | 5 |
| 7.295 | -2.200 | 1.00 | 0.00 | BED ATOM | 193 | HEZ SER | 5 | 7.295 | -2.200 | 1.00 | 0.00 | BED ATOM | 112 | HEZ SER | 5 |
| 9.216 | -2.211 | 1.00 | 0.00 | BED ATOM | 194 | HA SER | 5 | 9.216 | -2.211 | 1.00 | 0.00 | BED ATOM | 113 | HA SER | 5 |
| 5.906 | -1.857 | 1.00 | 0.00 | BED ATOM | 195 | HB SER | 5 | 5.906 | -1.857 | 1.00 | 0.00 | BED ATOM | 114 | HB SER | 5 |
| 6.590 | -1.857 | 1.00 | 0.00 | BED ATOM | 196 | HB2 SER | 5 | 6.590 | -1.857 | 1.00 | 0.00 | BED ATOM | 115 | HB2 SER | 5 |
| 6.874 | -2.334 | 1.00 | 0.00 | BED ATOM | 197 | HEI SER | 5 | 6.874 | -2.334 | 1.00 | 0.00 | BED ATOM | 116 | HEI SER | 5 |
| 5.982 | -2.402 | 1.00 | 0.00 | BED ATOM | 198 | HEC SER | 5 | 5.982 | -2.402 | 1.00 | 0.00 | BED ATOM | 117 | HEC SER | 5 |
| 4.676 | -2.000 | 1.00 | 0.00 | BED ATOM | 199 | HEZ SER | 5 | 4.676 | -2.000 | 1.00 | 0.00 | BED ATOM | 120 | HEZ SER | 5 |
| 6.266 | -1.874 | 1.00 | 0.00 | BED ATOM | 200 | CD PRO | 5 | 6.266 | -1.874 | 1.00 | 0.00 | BED ATOM | 121 | CD PRO | 5 |
| 4.476 | -1.740 | 1.00 | 0.00 | BED ATOM | 201 | HB1 PRO | 5 | 4.476 | -1.740 | 1.00 | 0.00 | BED ATOM | 122 | HB1 PRO | 5 |
| 4.176 | -3.694 | 1.00 | 0.00 | BED ATOM | 202 | HB2 PRO | 5 | 4.176 | -3.694 | 1.00 | 0.00 | BED ATOM | 123 | HB2 PRO | 5 |
| 4.476 | -3.837 | 1.00 | 0.00 | BED ATOM | 203 | HEI PRO | 5 | 4.476 | -3.837 | 1.00 | 0.00 | BED ATOM | 124 | HEI PRO | 5 |
| 3.571 | -3.837 | 1.00 | 0.00 | BED ATOM | 204 | HEC PRO | 5 | 3.571 | -3.837 | 1.00 | 0.00 | BED ATOM | 125 | HEC PRO | 5 |
| 3.221 | -3.711 | 1.00 | 0.00 | BED ATOM | 205 | HEZ PRO | 5 | 3.221 | -3.711 | 1.00 | 0.00 | BED ATOM | 126 | HEZ PRO | 5 |
| 3.617 | -3.711 | 1.00 | 0.00 | BED ATOM | 206 | CB ARG | 9 | 3.617 | -3.711 | 1.00 | 0.00 | BED ATOM | 127 | CB ARG | 9 |
| 3.529 | -2.074 | 1.00 | 0.00 | BED ATOM | 207 | HBL ARG | 9 | 3.529 | -2.074 | 1.00 | 0.00 | BED ATOM | 128 | HBL ARG | 9 |
| 3.864 | -2.238 | 1.00 | 0.00 | BED ATOM | 208 | HBL PRO | 5 | 3.864 | -2.238 | 1.00 | 0.00 | BED ATOM | 129 | HBL PRO | 5 |
| 2.982 | -2.402 | 1.00 | 0.00 | BED ATOM | 209 | HBL2 ARG | 9 | 2.982 | -2.402 | 1.00 | 0.00 | BED ATOM | 130 | HBL2 ARG | 9 |
| 4.476 | -2.000 | 1.00 | 0.00 | BED ATOM | 210 | HBL2 PRO | 5 | 4.476 | -2.000 | 1.00 | 0.00 | BED ATOM | 131 | HBL2 PRO | 5 |
| 4.476 | -3.837 | 1.00 | 0.00 | BED ATOM | 211 | HBL2 SER | 5 | 4.476 | -3.837 | 1.00 | 0.00 | BED ATOM | 132 | HBL2 SER | 5 |
| 4.476 | -3.837 | 1.00 | 0.00 | BED ATOM | 212 | HN ARG | 9 | 4.476 | -3.837 | 1.00 | 0.00 | BED ATOM | 133 | HN ARG | 9 |
| 4.476 | -3.837 | 1.00 | 0.00 | BED ATOM | 213 | HN PRO | 5 | 4.476 | -3.837 | 1.00 | 0.00 | BED ATOM | 134 | HN PRO | 5 |
| 4.476 | -3.837 | 1.00 | 0.00 | BED ATOM | 214 | HN SER | 5 | 4.476 | -3.837 | 1.00 | 0.00 | BED ATOM | 135 | HN SER | 5 |
| 4.476 | -3.837 | 1.00 | 0.00 | BED ATOM | 215 | CD PRO | 5 | 4.476 | -3.837 | 1.00 | 0.00 | BED ATOM | 136 | CD PRO | 5 |
| 4.476 | -3.837 | 1.00 | 0.00 | BED ATOM | 216 | CD SER | 5 | 4.476 | -3.837 | 1.00 | 0.00 | BED ATOM | 137 | CD SER | 5 |
| 4.476 | -3.837 | 1.00 | 0.00 | BED ATOM | 217 | HBL2 PRO | 5 | 4.476 | -3.837 | 1.00 | 0.00 | BED ATOM | 138 | HBL2 PRO | 5 |
| 4.476 | -3.837 | 1.00 | 0.00 | BED ATOM | 218 | HBL2 SER | 5 | 4.476 | -3.837 | 1.00 | 0.00 | BED ATOM | 139 | HBL2 SER | 5 |
| 4.476 | -3.837 | 1.00 | 0.00 | BED ATOM | 219 | PRO | 5 | 4.476 | -3.837 | 1.00 | 0.00 | BED ATOM | 140 | PRO | 5 |
| 4.476 | -3.837 | 1.00 | 0.00 | BED ATOM | 220 | ARG | 9 | 4.476 | -3.837 | 1.00 | 0.00 | BED ATOM | 141 | ARG | 9 |
| 4.476 | -3.837 | 1.00 | 0.00 | BED ATOM | 221 | CD ARG | 9 | 4.476 | -3.837 | 1.00 | 0.00 | BED ATOM | 142 | CD ARG | 9 |
| 4.476 | -3.837 | 1.00 | 0.00 | BED ATOM | 222 | CB ARG | 9 | 4.476 | -3.837 | 1.00 | 0.00 | BED ATOM | 143 | CB ARG | 9 |
| 4.476 | -3.837 | 1.00 | 0.00 | BED ATOM | 223 | HBL ARG | 9 | 4.476 | -3.837 | 1.00 | 0.00 | BED ATOM | 144 | HBL ARG | 9 |
| 4.476 | -3.837 | 1.00 | 0.00 | BED ATOM | 224 | HBL PRO | 5 | 4.476 | -3.837 | 1.00 | 0.00 | BED ATOM | 145 | HBL PRO | 5 |
| 4.476 | -3.837 | 1.00 | 0.00 | BED ATOM | 225 | HBL2 ARG | 9 | 4.476 | -3.837 | 1.00 | 0.00 | BED ATOM | 146 | HBL2 ARG | 9 |
| 4.476 | -3.837 | 1.00 | 0.00 | BED ATOM | 226 | HBL2 PRO | 5 | 4.476 | -3.837 | 1.00 | 0.00 | BED ATOM | 147 | HBL2 PRO | 5 |
| 4.476 | -3.837 | 1.00 | 0.00 | BED ATOM | 227 | HBL2 SER | 5 | 4.476 | -3.837 | 1.00 | 0.00 | BED ATOM | 148 | HBL2 SER | 5 |
| 4.476 | -3.837 | 1.00 | 0.00 | BED ATOM | 228 | PRO | 5 | 4.476 | -3.837 | 1.00 | 0.00 | BED ATOM | 149 | PRO | 5 |
| 4.476 | -3.837 | 1.00 | 0.00 | BED ATOM | 229 | ARG | 9 | 4.476 | -3.837 | 1.00 | 0.00 | BED ATOM | 150 | ARG | 9 |
| 4.476 | -3.837 | 1.00 | 0.00 | BED ATOM | 230 | CD PRO | 5 | 4.476 | -3.837 | 1.00 | 0.00 | BED ATOM | 151 | CD PRO | 5 |
| 4.476 | -3.837 | 1.00 | 0.00 | BED ATOM | 231 | CB PRO | 5 | 4.476 | -3.837 | 1.00 | 0.00 | BED ATOM | 152 | CB PRO | 5 |
| 4.476 | -3.837 | 1.00 | 0.00 | BED ATOM | 232 | HBL2 PRO | 5 | 4.476 | -3.837 | 1.00 | 0.00 | BED ATOM | 153 | HBL2 PRO | 5 |
| 4.476 | -3.837 | 1.00 | 0.00 | BED ATOM | 233 | HBL2 SER | 5 | 4.476 | -3.837 | 1.00 | 0.00 | BED ATOM | 154 | HBL2 SER | 5 |
| 4.476 | -3.837 | 1.00 | 0.00 | BED ATOM | 234 | PRO | 5 | 4.476 | -3.837 | 1.00 | 0.00 | BED ATOM | 155 | PRO | 5 |
| 4.476 | -3.837 | 1.00 | 0.00 | BED ATOM | 235 | ARG | 9 | 4.476 | -3.837 | 1.00 | 0.00 | BED ATOM | 156 | ARG | 9 |
| 4.476 | -3.837 | 1.00 | 0.00 | BED ATOM | 236 | CD SER | 5 | 4.476 | -3.837 | 1.00 | 0.00 | BED ATOM | 157 | CD SER | 5 |
| 4.476 | -3.837 | 1.00 | 0. | | | | | | | | | | | | |

| | | | |
|----------|-----|----|-----|
| 89D ATOM | 159 | HN | ARG |
| 89D ATOM | 160 | HN | ARG |
| 89D ATOM | 161 | HN | ARG |
| 89D ATOM | 162 | C | ARG |
| 89D ATOM | 163 | O | ARG |
| 89D ATOM | 164 | N | ASP |
| 89D ATOM | 165 | H | ASP |
| 89D ATOM | 166 | C | ASP |
| 89D ATOM | 167 | H | ASP |
| 89D ATOM | 168 | G | ASP |
| 89D ATOM | 169 | F | ASP |
| 89D ATOM | 170 | D | ASP |
| 89D ATOM | 171 | C | ASP |
| 89D ATOM | 172 | C | ASP |
| 89D ATOM | 173 | O | ASP |
| 89D ATOM | 174 | C | ASP |
| 89D ATOM | 175 | O | ASP |
| 89D ATOM | 176 | C | ASP |
| 89D ATOM | 177 | C | ASP |
| 89D ATOM | 178 | C | PRO |
| 89D ATOM | 179 | C | PRO |
| 89D ATOM | 180 | F | PRO |
| 89D ATOM | 181 | R | PRO |
| 89D ATOM | 182 | C | PRO |
| 89D ATOM | 183 | G | PRO |
| 89D ATOM | 184 | H | PRO |
| 89D ATOM | 185 | C | PRO |
| 89D ATOM | 186 | H | PRO |
| 89D ATOM | 187 | H | PRO |
| 89D ATOM | 188 | C | PRO |
| 89D ATOM | 189 | O | PRO |
| 89D ATOM | 190 | N | ASP |
| 89D ATOM | 191 | H | ASP |
| 89D ATOM | 192 | C | ASP |
| 89D ATOM | 193 | H | ASP |
| 89D ATOM | 194 | C | ASP |
| 89D ATOM | 195 | H | ASP |
| 89D ATOM | 196 | H | ASP |
| 89D ATOM | 197 | C | ASP |
| 89D ATOM | 198 | O | ASP |
| 89D ATOM | 199 | O | ASP |
| 89D ATOM | 200 | C | ASP |
| 89D ATOM | 201 | O | ASP |
| 89D ATOM | 202 | N | GLN |
| 89D ATOM | 203 | H | GLN |
| 89D ATOM | 204 | C | GLN |
| 89D ATOM | 205 | N | GLN |
| 89D ATOM | 206 | G | GLN |
| 89D ATOM | 207 | H | GLN |
| 89D ATOM | 208 | G | GLN |
| 89D ATOM | 209 | C | GLN |
| 89D ATOM | 210 | H | GLN |
| 89D ATOM | 211 | H | GLN |
| 89D ATOM | 212 | C | GLN |
| 89D ATOM | 213 | N | GLN |
| 89D ATOM | 214 | E | GLN |
| 89D ATOM | 215 | H | GLN |
| 89D ATOM | 216 | E | GLN |
| 89D ATOM | 217 | H | GLN |
| 89D ATOM | 218 | N | GLN |
| 89D ATOM | 219 | C | GLN |
| 89D ATOM | 220 | H | GLN |
| 89D ATOM | 221 | C | LEU |
| 89D ATOM | 222 | H | LEU |
| 89D ATOM | 223 | C | LEU |
| 89D ATOM | 224 | S | LEU |
| 89D ATOM | 225 | H | LEU |
| 89D ATOM | 226 | C | LEU |
| 89D ATOM | 227 | H | LEU |
| 89D ATOM | 228 | C | LEU |
| 89D ATOM | 229 | H | LEU |
| 89D ATOM | 230 | D | LEU |
| 89D ATOM | 231 | H | LEU |
| 89D ATOM | 232 | C | LEU |
| 89D ATOM | 233 | H | LEU |
| 89D ATOM | 234 | D | LEU |
| 89D ATOM | 235 | C | LEU |
| 89D ATOM | 236 | C | LEU |
| 89D ATOM | 237 | N | LEU |
| 89D ATOM | 238 | N | LEU |
| 89D ATOM | 239 | H | LEU |
| 89D ATOM | 240 | C | TYR |
| 89D ATOM | 241 | H | TYR |
| 89D ATOM | 242 | C | TYR |
| 89D ATOM | 243 | H | TYR |
| 89D ATOM | 244 | H | TYR |
| 89D ATOM | 245 | C | TYR |
| 89D ATOM | 246 | C | TYR |
| 89D ATOM | 247 | H | TYR |
| 89D ATOM | 248 | H | TYR |
| 89D ATOM | 249 | O | TYR |
| 89D ATOM | 250 | O | TYR |
| 89D ATOM | 251 | O | TYR |
| 89D ATOM | 252 | C | TYR |

REPLACEMENT SHEET

| | | | | | | | | | | | | | | | | | | | | | | | | | | |
|-------|---------|------|------|----------|-----|---------|----|--------|--------|-------|------|------|----------|-----|----------|----|-------|--------|---------|------|------|----------|-----|---------|----|---------|
| 7.249 | -6.837 | 1.00 | 0.00 | BED ATOM | 293 | H2P TPR | 15 | 9.275 | 8.431 | 2.377 | 1.00 | 0.00 | BED ATOM | 347 | HE22 TLE | 21 | 3.319 | 12.844 | -9.465 | 1.00 | 0.00 | BED ATOM | 441 | HL1 LYS | 26 | -1.215 |
| 7.246 | -7.111 | 1.00 | 0.00 | BED ATOM | 294 | CG TPR | 15 | 11.284 | 9.603 | 2.603 | 1.00 | 0.00 | BED ATOM | 348 | HE22 TLE | 21 | 3.073 | 13.385 | -9.384 | 1.00 | 0.00 | BED ATOM | 442 | HL2 LYS | 26 | -0.010 |
| 7.246 | -7.706 | 1.00 | 0.00 | BED ATOM | 295 | CH TPR | 15 | 10.908 | 7.915 | 3.053 | 1.00 | 0.00 | BED ATOM | 349 | CDN TLE | 21 | 3.222 | 13.461 | -8.710 | 1.00 | 0.00 | BED ATOM | 443 | HE3 LYS | 26 | -0.558 |
| 7.246 | -7.732 | 1.00 | 0.00 | BED ATOM | 296 | HH TPR | 15 | 10.572 | 6.130 | 4.000 | 1.00 | 0.00 | BED ATOM | 350 | HD1 TLE | 21 | 3.805 | 12.449 | -10.199 | 1.00 | 0.00 | BED ATOM | 444 | C LYS | 26 | -4.673 |
| 7.246 | -7.819 | 1.00 | 0.00 | BED ATOM | 297 | C TPR | 15 | 10.859 | 5.225 | 3.384 | 1.00 | 0.00 | BED ATOM | 351 | HD2 TLE | 21 | 2.264 | 11.073 | -5.468 | 1.00 | 0.00 | BED ATOM | 445 | N LYS | 26 | -5.762 |
| 7.246 | -7.869 | 1.00 | 0.00 | BED ATOM | 298 | S TPR | 15 | 9.778 | 6.000 | 0.051 | 1.00 | 0.00 | BED ATOM | 352 | HD3 TLE | 21 | 3.075 | 10.991 | -6.036 | 1.00 | 0.00 | BED ATOM | 446 | IN LYS | 26 | -4.315 |
| 7.246 | -7.911 | 1.00 | 0.00 | BED ATOM | 299 | NE TPR | 15 | 11.641 | 6.371 | 1.422 | 1.00 | 0.00 | BED ATOM | 353 | C TLE | 21 | 1.969 | 12.118 | -4.732 | 1.00 | 0.00 | BED ATOM | 447 | HN SER | 27 | -3.439 |
| 7.246 | -7.950 | 1.00 | 0.00 | BED ATOM | 300 | NI SER | 16 | 11.465 | 6.024 | 1.044 | 1.00 | 0.00 | BED ATOM | 354 | O TLE | 21 | 0.869 | 12.109 | -4.493 | 1.00 | 0.00 | BED ATOM | 448 | ON SER | 27 | -5.204 |
| 7.246 | -7.986 | 1.00 | 0.00 | BED ATOM | 301 | HA SER | 16 | 11.449 | 6.808 | 1.991 | 1.00 | 0.00 | BED ATOM | 355 | R N LEP | 22 | 3.433 | 13.157 | -4.156 | 1.00 | 0.00 | BED ATOM | 449 | RA SER | 27 | -6.104 |
| 7.246 | -8.020 | 1.00 | 0.00 | BED ATOM | 302 | GA SER | 16 | 11.448 | 8.824 | 2.004 | 1.00 | 0.00 | BED ATOM | 356 | R N LEP | 22 | 3.125 | 13.100 | -3.091 | 1.00 | 0.00 | BED ATOM | 450 | RD SER | 27 | -4.932 |
| 7.246 | -8.058 | 1.00 | 0.00 | BED ATOM | 303 | GB SER | 16 | 11.448 | 9.307 | 2.229 | 1.00 | 0.00 | BED ATOM | 357 | CA LEP | 22 | 6.688 | 14.953 | -4.976 | 1.00 | 0.00 | BED ATOM | 451 | HB1 SER | 27 | -3.629 |
| 7.246 | -8.090 | 1.00 | 0.00 | BED ATOM | 304 | HE1 TLE | 21 | 12.105 | 7.807 | 2.929 | 1.00 | 0.00 | BED ATOM | 358 | GB LEP | 22 | 4.491 | 14.710 | -4.404 | 1.00 | 0.00 | BED ATOM | 452 | HB2 SER | 27 | -5.207 |
| 7.246 | -8.122 | 1.00 | 0.00 | BED ATOM | 305 | HE2 TLE | 21 | 12.220 | 11.692 | 1.100 | 1.00 | 0.00 | BED ATOM | 359 | CB LEP | 22 | 4.491 | 14.710 | -4.404 | 1.00 | 0.00 | BED ATOM | 453 | HG SER | 27 | -4.197 |
| 7.246 | -8.154 | 1.00 | 0.00 | BED ATOM | 306 | HE3 TLE | 21 | 12.220 | 11.692 | 1.100 | 1.00 | 0.00 | BED ATOM | 360 | HE1 LEP | 22 | 4.491 | 14.710 | -4.404 | 1.00 | 0.00 | BED ATOM | 454 | HG2 SER | 27 | -3.746 |
| 7.246 | -8.186 | 1.00 | 0.00 | BED ATOM | 307 | HE2 SER | 16 | 11.317 | 11.317 | 1.000 | 1.00 | 0.00 | BED ATOM | 361 | HE2 LEP | 22 | 2.778 | 13.100 | -6.006 | 1.00 | 0.00 | BED ATOM | 455 | ON SER | 27 | -5.591 |
| 7.246 | -8.217 | 1.00 | 0.00 | BED ATOM | 308 | HE3 SER | 16 | 11.317 | 11.317 | 1.000 | 1.00 | 0.00 | BED ATOM | 362 | HE2 TLE | 22 | 1.722 | 13.161 | -3.950 | 1.00 | 0.00 | BED ATOM | 456 | O SER | 27 | -5.862 |
| 7.246 | -8.249 | 1.00 | 0.00 | BED ATOM | 309 | HE1 TLE | 21 | 10.182 | 1.161 | 1.000 | 0.00 | 0.00 | BED ATOM | 363 | CO TLE | 21 | 2.378 | 14.131 | -3.380 | 1.00 | 0.00 | BED ATOM | 457 | HA SER | 27 | -5.877 |
| 7.246 | -8.281 | 1.00 | 0.00 | BED ATOM | 310 | HE2 TLE | 21 | 10.182 | 1.161 | 1.000 | 0.00 | 0.00 | BED ATOM | 364 | HE1 LEP | 22 | 2.375 | 14.131 | -3.380 | 1.00 | 0.00 | BED ATOM | 458 | HL1 SER | 27 | -5.215 |
| 7.246 | -8.313 | 1.00 | 0.00 | BED ATOM | 311 | HE3 TLE | 21 | 10.182 | 1.161 | 1.000 | 0.00 | 0.00 | BED ATOM | 365 | HE1 LEP | 22 | 2.375 | 14.131 | -3.380 | 1.00 | 0.00 | BED ATOM | 459 | HL2 SER | 27 | -5.663 |
| 7.246 | -8.345 | 1.00 | 0.00 | BED ATOM | 312 | CA TLE | 21 | 10.182 | 1.161 | 1.000 | 0.00 | 0.00 | BED ATOM | 366 | HE1 LEP | 22 | 2.375 | 14.131 | -3.380 | 1.00 | 0.00 | BED ATOM | 460 | HL3 SER | 28 | -5.595 |
| 7.246 | -8.376 | 1.00 | 0.00 | BED ATOM | 313 | CH TLE | 21 | 10.182 | 1.161 | 1.000 | 0.00 | 0.00 | BED ATOM | 367 | HE1 LEP | 22 | 2.375 | 14.131 | -3.380 | 1.00 | 0.00 | BED ATOM | 461 | HL3 SER | 28 | -5.125 |
| 7.246 | -8.408 | 1.00 | 0.00 | BED ATOM | 314 | CB TLE | 21 | 10.182 | 1.161 | 1.000 | 0.00 | 0.00 | BED ATOM | 368 | HE1 LEP | 22 | 2.375 | 14.131 | -3.380 | 1.00 | 0.00 | BED ATOM | 462 | HL1 SER | 28 | -4.733 |
| 7.246 | -8.440 | 1.00 | 0.00 | BED ATOM | 315 | CG TLE | 21 | 10.182 | 1.161 | 1.000 | 0.00 | 0.00 | BED ATOM | 369 | HE1 LEP | 22 | 2.375 | 14.131 | -3.380 | 1.00 | 0.00 | BED ATOM | 463 | HL2 SER | 27 | -4.207 |
| 7.246 | -8.472 | 1.00 | 0.00 | BED ATOM | 316 | CC TLE | 21 | 10.182 | 1.161 | 1.000 | 0.00 | 0.00 | BED ATOM | 370 | HE1 LEP | 22 | 2.375 | 14.131 | -3.380 | 1.00 | 0.00 | BED ATOM | 464 | HL3 SER | 27 | -3.817 |
| 7.246 | -8.504 | 1.00 | 0.00 | BED ATOM | 317 | CH TLE | 21 | 10.182 | 1.161 | 1.000 | 0.00 | 0.00 | BED ATOM | 371 | HE2 LEP | 21 | 0.700 | 10.884 | -1.880 | 1.00 | 0.00 | BED ATOM | 465 | NN LHS | 28 | -5.542 |
| 7.246 | -8.536 | 1.00 | 0.00 | BED ATOM | 318 | CA TLE | 21 | 10.182 | 1.161 | 1.000 | 0.00 | 0.00 | BED ATOM | 372 | HE2 LEP | 21 | 2.375 | 14.131 | -3.380 | 1.00 | 0.00 | BED ATOM | 466 | NN HIS | 28 | -5.446 |
| 7.246 | -8.568 | 1.00 | 0.00 | BED ATOM | 319 | CB TLE | 21 | 10.182 | 1.161 | 1.000 | 0.00 | 0.00 | BED ATOM | 373 | HE2 LEP | 21 | 2.375 | 14.131 | -3.380 | 1.00 | 0.00 | BED ATOM | 467 | CDP HIS | 28 | -5.066 |
| 7.246 | -8.600 | 1.00 | 0.00 | BED ATOM | 320 | CG TLE | 21 | 10.182 | 1.161 | 1.000 | 0.00 | 0.00 | BED ATOM | 374 | N GLN | 23 | 2.201 | 9.744 | -1.985 | 1.00 | 0.00 | BED ATOM | 468 | CDP HIS | 28 | -5.717 |
| 7.246 | -8.632 | 1.00 | 0.00 | BED ATOM | 321 | CH TLE | 21 | 10.182 | 1.161 | 1.000 | 0.00 | 0.00 | BED ATOM | 375 | HE1 GLN | 23 | 3.107 | 13.166 | -1.917 | 1.00 | 0.00 | BED ATOM | 469 | CDL HIS | 28 | -6.032 |
| 7.246 | -8.664 | 1.00 | 0.00 | BED ATOM | 322 | HE1 TLE | 21 | 10.182 | 1.161 | 1.000 | 0.00 | 0.00 | BED ATOM | 376 | HE1 GLN | 23 | 1.941 | 12.456 | -1.917 | 1.00 | 0.00 | BED ATOM | 470 | HE1 HIS | 28 | -6.314 |
| 7.246 | -8.696 | 1.00 | 0.00 | BED ATOM | 323 | HE2 TLE | 21 | 10.182 | 1.161 | 1.000 | 0.00 | 0.00 | BED ATOM | 377 | HE1 GLN | 23 | 1.828 | 12.044 | -1.917 | 1.00 | 0.00 | BED ATOM | 471 | HE2 HIS | 28 | -6.119 |
| 7.246 | -8.728 | 1.00 | 0.00 | BED ATOM | 324 | HE3 TLE | 21 | 10.182 | 1.161 | 1.000 | 0.00 | 0.00 | BED ATOM | 378 | HE1 GLN | 23 | 3.118 | 10.850 | -1.917 | 1.00 | 0.00 | BED ATOM | 472 | HE2 HIS | 28 | -6.350 |
| 7.246 | -8.760 | 1.00 | 0.00 | BED ATOM | 325 | HE1 SER | 16 | 9.593 | 13.346 | 1.000 | 0.00 | 0.00 | BED ATOM | 379 | HE1 GLN | 23 | 9.536 | 13.951 | -1.917 | 1.00 | 0.00 | BED ATOM | 473 | C HIS | 28 | -7.364 |
| 7.246 | -8.792 | 1.00 | 0.00 | BED ATOM | 326 | HE2 SER | 16 | 9.593 | 13.346 | 1.000 | 0.00 | 0.00 | BED ATOM | 380 | HE1 GLN | 23 | 9.536 | 13.951 | -1.917 | 1.00 | 0.00 | BED ATOM | 474 | O HIS | 28 | -7.797 |
| 7.246 | -8.824 | 1.00 | 0.00 | BED ATOM | 327 | HE3 SER | 16 | 9.593 | 13.346 | 1.000 | 0.00 | 0.00 | BED ATOM | 381 | HE1 GLN | 23 | 9.536 | 13.951 | -1.917 | 1.00 | 0.00 | BED ATOM | 475 | N HIS | 28 | -8.215 |
| 7.246 | -8.856 | 1.00 | 0.00 | BED ATOM | 328 | HE1 TLE | 21 | 10.182 | 1.161 | 1.000 | 0.00 | 0.00 | BED ATOM | 382 | HE1 GLN | 23 | 9.536 | 13.951 | -1.917 | 1.00 | 0.00 | BED ATOM | 476 | HE1 LYS | 26 | -8.660 |
| 7.246 | -8.888 | 1.00 | 0.00 | BED ATOM | 329 | HE2 TLE | 21 | 10.182 | 1.161 | 1.000 | 0.00 | 0.00 | BED ATOM | 383 | HE1 GLN | 23 | 9.536 | 13.951 | -1.917 | 1.00 | 0.00 | BED ATOM | 477 | HE2 LYS | 26 | -8.740 |
| 7.246 | -9.020 | 1.00 | 0.00 | BED ATOM | 330 | HE3 TLE | 21 | 10.182 | 1.161 | 1.000 | 0.00 | 0.00 | BED ATOM | 384 | HE1 GLN | 23 | 9.536 | 13.951 | -1.917 | 1.00 | 0.00 | BED ATOM | 478 | HE3 LYS | 26 | -9.129 |
| 7.246 | -9.152 | 1.00 | 0.00 | BED ATOM | 331 | HE1 SER | 20 | 9.593 | 12.423 | 1.000 | 0.00 | 0.00 | BED ATOM | 385 | HE1 GLN | 23 | 9.536 | 13.951 | -1.917 | 1.00 | 0.00 | BED ATOM | 479 | HE1 HIS | 26 | -9.512 |
| 7.246 | -9.284 | 1.00 | 0.00 | BED ATOM | 332 | HE2 SER | 20 | 9.593 | 12.423 | 1.000 | 0.00 | 0.00 | BED ATOM | 386 | HE1 GLN | 23 | 9.536 | 13.951 | -1.917 | 1.00 | 0.00 | BED ATOM | 480 | HE2 HIS | 26 | -9.893 |
| 7.246 | -9.416 | 1.00 | 0.00 | BED ATOM | 333 | HE3 SER | 20 | 9.593 | 12.423 | 1.000 | 0.00 | 0.00 | BED ATOM | 387 | HE1 GLN | 23 | 9.536 | 13.951 | -1.917 | 1.00 | 0.00 | BED ATOM | 481 | HE3 HIS | 26 | -10.272 |
| 7.246 | -9.548 | 1.00 | 0.00 | BED ATOM | 334 | HE1 TLE | 21 | 10.182 | 1.161 | 1.000 | 0.00 | 0.00 | BED ATOM | 388 | HE1 GLN | 23 | 9.536 | 13.951 | -1.917 | 1.00 | 0.00 | BED ATOM | 482 | HE1 LYS | 26 | -10.651 |
| 7.246 | -9.680 | 1.00 | 0.00 | BED ATOM | 335 | HE2 TLE | 21 | 10.182 | 1.161 | 1.000 | 0.00 | 0.00 | BED ATOM | 389 | HE1 GLN | 23 | 9.536 | 13.951 | -1.917 | 1.00 | 0.00 | BED ATOM | 483 | HE2 LYS | 26 | -11.030 |
| 7.246 | -9.812 | 1.00 | 0.00 | BED ATOM | 336 | HE3 TLE | 21 | 10.182 | 1.161 | 1.000 | 0.00 | 0.00 | BED ATOM | 390 | HE1 GLN | 23 | 9.536 | 13.951 | -1.917 | 1.00 | 0.00 | BED ATOM | 484 | HE3 LYS | 26 | -11.409 |
| 7.246 | -10.044 | 1.00 | 0.00 | BED ATOM | 337 | HE1 SER | 20 | 9.593 | 12.423 | 1.000 | 0.00 | 0.00 | BED ATOM | 391 | HE1 GLN | 23 | 9 | | | | | | | | | |

REPLACEMENT SHEET

| | | | | | | | | | | | | | | | | | |
|-------|--------|------|------|----------|-----|---------|----|---------|-------|---------|------|------|----------|-----|----------|----|---------|
| 1.938 | 1.963 | 1.00 | 0.00 | BED ATOM | 535 | C TRP | 32 | -10.855 | 5.374 | 5.333 | 1.00 | 0.00 | BED ATOM | 629 | H022 VAL | 38 | -13.457 |
| 5.382 | -2.797 | 1.00 | 0.00 | BED ATOM | 536 | O TRP | 32 | -11.199 | 4.994 | 7.020 | 1.00 | 0.00 | BED ATOM | 723 | H02 PRO | 44 | -17.551 |
| 4.752 | -3.797 | 1.00 | 0.00 | BED ATOM | 537 | N PRO | 33 | -10.636 | 6.629 | 6.533 | 1.00 | 0.00 | BED ATOM | 724 | C PRO | 44 | -18.125 |
| 4.574 | -3.618 | 1.00 | 0.00 | BED ATOM | 538 | CA PRO | 33 | -10.800 | 6.481 | 6.533 | 1.00 | 0.00 | BED ATOM | 631 | C VAL | 38 | -10.518 |
| 3.497 | -1.493 | 1.00 | 0.00 | BED ATOM | 539 | HA PRO | 33 | -11.693 | 6.473 | 8.511 | 1.00 | 0.00 | BED ATOM | 632 | O VAL | 38 | -10.518 |
| 3.255 | -1.599 | 1.00 | 0.00 | BED ATOM | 540 | CB PRO | 33 | -10.947 | 6.488 | 8.051 | 1.00 | 0.00 | BED ATOM | 633 | N LYS | 39 | -11.349 |
| 3.057 | 0.017 | 1.00 | 0.00 | BED ATOM | 541 | HB1 PRO | 33 | -10.191 | 7.412 | 7.609 | 1.00 | 0.00 | BED ATOM | 634 | CA LYS | 39 | -12.205 |
| 3.357 | -0.341 | 1.00 | 0.00 | BED ATOM | 542 | HB2 PRO | 33 | -11.926 | 8.717 | 8.715 | 1.00 | 0.00 | BED ATOM | 635 | DA LYS | 39 | -11.005 |
| 1.846 | 0.219 | 1.00 | 0.00 | BED ATOM | 543 | CG PRO | 33 | -10.771 | 8.306 | -8.574 | 1.00 | 0.00 | BED ATOM | 637 | CB LYS | 39 | -11.299 |
| 4.396 | 0.695 | 1.00 | 0.00 | BED ATOM | 544 | HG1 PRO | 33 | -11.713 | 8.666 | -10.216 | 1.00 | 0.00 | BED ATOM | 638 | HBL LYS | 39 | -10.419 |
| 4.744 | 1.048 | 1.00 | 0.00 | BED ATOM | 545 | HG2 PRO | 33 | -10.075 | 8.205 | -10.714 | 1.00 | 0.00 | BED ATOM | 639 | HB2 LYS | 39 | -11.511 |
| 4.498 | 1.505 | 1.00 | 0.00 | BED ATOM | 546 | CD PRO | 33 | -10.223 | 8.633 | -10.569 | 1.00 | 0.00 | BED ATOM | 640 | CG LYS | 39 | -12.452 |
| 6.219 | 0.337 | 1.00 | 0.00 | BED ATOM | 547 | HD1 PRO | 33 | -10.632 | 7.772 | -10.569 | 1.00 | 0.00 | BED ATOM | 641 | HGL LYS | 39 | -12.490 |
| 5.566 | -0.355 | 1.00 | 0.00 | BED ATOM | 548 | HD2 PRO | 33 | -10.165 | 7.450 | -9.664 | 1.00 | 0.00 | BED ATOM | 642 | HGL LYS | 39 | -13.177 |
| 6.219 | 0.304 | 1.00 | 0.00 | BED ATOM | 549 | C PRO | 33 | -9.996 | 8.241 | -11.222 | 1.00 | 0.00 | BED ATOM | 643 | CD LYS | 39 | -11.947 |
| 2.933 | -2.312 | 1.00 | 0.00 | BED ATOM | 550 | N PRO | 33 | -9.887 | 8.108 | -11.222 | 1.00 | 0.00 | BED ATOM | 644 | DA LYS | 39 | -12.413 |
| 2.612 | 0.200 | 1.00 | 0.00 | BED ATOM | 551 | PHE | 34 | -9.472 | 8.618 | -11.222 | 1.00 | 0.00 | BED ATOM | 645 | HDS PRO | 39 | -10.888 |
| 2.689 | -0.225 | 1.00 | 0.00 | BED ATOM | 552 | SAW | 34 | -9.558 | 8.642 | -11.160 | 1.00 | 0.00 | BED ATOM | 646 | CE LYS | 39 | -12.326 |
| 1.805 | -0.203 | 1.00 | 0.00 | BED ATOM | 553 | CA PRO | 34 | -7.256 | 8.659 | -11.222 | 1.00 | 0.00 | BED ATOM | 647 | HE1 LYS | 39 | -12.074 |
| 5.659 | -0.303 | 1.00 | 0.00 | BED ATOM | 554 | MA PRO | 34 | -6.597 | 8.725 | -11.166 | 1.00 | 0.00 | BED ATOM | 648 | HE2 LYS | 39 | -13.060 |
| 5.324 | -0.617 | 1.00 | 0.00 | BED ATOM | 555 | HA PRO | 34 | -7.775 | 8.328 | -12.030 | 1.00 | 0.00 | BED ATOM | 649 | SD LYS | 39 | -13.560 |
| 6.968 | 1.565 | 1.00 | 0.00 | BED ATOM | 556 | HE1 PRO | 34 | -5.198 | 8.650 | -11.222 | 1.00 | 0.00 | BED ATOM | 650 | HE2 LYS | 39 | -13.962 |
| 2.303 | 2.779 | 1.00 | 0.00 | BED ATOM | 557 | HB1 PRO | 34 | -6.228 | 8.540 | -11.222 | 1.00 | 0.00 | BED ATOM | 651 | HB2 LYS | 39 | -14.307 |
| 4.944 | 1.335 | 1.00 | 0.00 | BED ATOM | 558 | CD PRO | 34 | -6.085 | 8.531 | -11.222 | 1.00 | 0.00 | BED ATOM | 652 | HE1 LYS | 39 | -14.772 |
| 5.829 | -0.151 | 1.00 | 0.00 | BED ATOM | 559 | CO PRO | 34 | -6.085 | 8.531 | -11.222 | 1.00 | 0.00 | BED ATOM | 653 | CO LYS | 39 | -14.772 |
| 4.098 | 2.122 | 1.00 | 0.00 | BED ATOM | 560 | CH PRO | 34 | -7.303 | 8.689 | -11.222 | 1.00 | 0.00 | BED ATOM | 654 | CB LYS | 39 | -14.772 |
| 4.316 | 0.226 | 1.00 | 0.00 | BED ATOM | 561 | COP PRO | 34 | -5.663 | 8.689 | -11.222 | 1.00 | 0.00 | BED ATOM | 655 | N LYS | 39 | -14.772 |
| 5.622 | 0.203 | 1.00 | 0.00 | BED ATOM | 562 | HO2 PRO | 34 | -5.674 | 8.689 | -11.222 | 1.00 | 0.00 | BED ATOM | 656 | HE1 LYS | 39 | -14.772 |
| 5.324 | -0.617 | 1.00 | 0.00 | BED ATOM | 563 | CSL PRO | 34 | -7.375 | 8.689 | -11.222 | 1.00 | 0.00 | BED ATOM | 657 | CS LYS | 39 | -14.772 |
| 6.968 | 1.565 | 1.00 | 0.00 | BED ATOM | 564 | HE1 PRO | 34 | -7.767 | 8.689 | -11.222 | 1.00 | 0.00 | BED ATOM | 658 | HE2 PRO | 34 | -11.066 |
| 2.303 | 2.779 | 1.00 | 0.00 | BED ATOM | 565 | CB2 PRO | 34 | -5.052 | 8.419 | -11.222 | 1.00 | 0.00 | BED ATOM | 659 | CH2 LYS | 39 | -14.772 |
| 4.098 | -0.151 | 1.00 | 0.00 | BED ATOM | 566 | CD2 PRO | 34 | -6.409 | 8.419 | -11.222 | 1.00 | 0.00 | BED ATOM | 660 | HE2 LYS | 39 | -14.772 |
| 5.829 | -0.151 | 1.00 | 0.00 | BED ATOM | 567 | CB PRO | 34 | -6.607 | 8.419 | -11.222 | 1.00 | 0.00 | BED ATOM | 661 | HE1 LYS | 39 | -14.772 |
| 4.098 | -0.151 | 1.00 | 0.00 | BED ATOM | 568 | CH PRO | 34 | -6.753 | 8.419 | -11.222 | 1.00 | 0.00 | BED ATOM | 662 | HE2 LYS | 39 | -14.772 |
| 5.829 | -0.151 | 1.00 | 0.00 | BED ATOM | 569 | CG PRO | 34 | -7.150 | 8.419 | -11.222 | 1.00 | 0.00 | BED ATOM | 663 | CB LYS | 39 | -14.772 |
| 4.098 | -0.151 | 1.00 | 0.00 | BED ATOM | 570 | MA PRO | 34 | -6.653 | 8.419 | -11.222 | 1.00 | 0.00 | BED ATOM | 664 | HE1 LYS | 39 | -14.772 |
| 5.829 | -0.151 | 1.00 | 0.00 | BED ATOM | 571 | HA PRO | 34 | -7.624 | 8.419 | -11.222 | 1.00 | 0.00 | BED ATOM | 665 | HE2 LYS | 39 | -14.772 |
| 4.098 | -0.151 | 1.00 | 0.00 | BED ATOM | 572 | HN PRO | 34 | -7.624 | 8.419 | -11.222 | 1.00 | 0.00 | BED ATOM | 666 | HA LYS | 39 | -14.772 |
| 5.829 | -0.151 | 1.00 | 0.00 | BED ATOM | 573 | CA PRO | 34 | -7.845 | 8.419 | -11.222 | 1.00 | 0.00 | BED ATOM | 667 | HB1 LYS | 39 | -14.772 |
| 4.098 | -0.151 | 1.00 | 0.00 | BED ATOM | 574 | HA PRO | 34 | -6.930 | 8.419 | -11.222 | 1.00 | 0.00 | BED ATOM | 668 | HB2 LYS | 39 | -14.772 |
| 5.829 | -0.151 | 1.00 | 0.00 | BED ATOM | 575 | CB PRO | 34 | -7.845 | 8.419 | -11.222 | 1.00 | 0.00 | BED ATOM | 669 | HE1 LYS | 39 | -14.772 |
| 4.098 | -0.151 | 1.00 | 0.00 | BED ATOM | 576 | HE1 PRO | 34 | -7.845 | 8.419 | -11.222 | 1.00 | 0.00 | BED ATOM | 670 | HE2 PRO | 34 | -11.225 |
| 5.829 | -0.151 | 1.00 | 0.00 | BED ATOM | 577 | HE2 PRO | 34 | -7.845 | 8.419 | -11.222 | 1.00 | 0.00 | BED ATOM | 671 | HE1 LYS | 39 | -14.772 |
| 4.098 | -0.151 | 1.00 | 0.00 | BED ATOM | 578 | HE1 PRO | 34 | -7.845 | 8.419 | -11.222 | 1.00 | 0.00 | BED ATOM | 672 | HE2 LYS | 39 | -14.772 |
| 5.829 | -0.151 | 1.00 | 0.00 | BED ATOM | 579 | HE2 PRO | 34 | -7.845 | 8.419 | -11.222 | 1.00 | 0.00 | BED ATOM | 673 | HE1 LYS | 39 | -14.772 |
| 4.098 | -0.151 | 1.00 | 0.00 | BED ATOM | 580 | HE1 PRO | 34 | -7.845 | 8.419 | -11.222 | 1.00 | 0.00 | BED ATOM | 674 | HE2 LYS | 39 | -14.772 |
| 5.829 | -0.151 | 1.00 | 0.00 | BED ATOM | 581 | HE2 PRO | 34 | -7.845 | 8.419 | -11.222 | 1.00 | 0.00 | BED ATOM | 675 | HE1 LYS | 39 | -14.772 |
| 4.098 | -0.151 | 1.00 | 0.00 | BED ATOM | 582 | HE1 PRO | 34 | -7.845 | 8.419 | -11.222 | 1.00 | 0.00 | BED ATOM | 676 | HE2 LYS | 39 | -14.772 |
| 5.829 | -0.151 | 1.00 | 0.00 | BED ATOM | 583 | HE2 PRO | 34 | -7.845 | 8.419 | -11.222 | 1.00 | 0.00 | BED ATOM | 677 | HE1 LYS | 39 | -14.772 |
| 4.098 | -0.151 | 1.00 | 0.00 | BED ATOM | 584 | HE2 MET | 35 | -4.294 | 8.419 | -11.222 | 1.00 | 0.00 | BED ATOM | 678 | HE1 LYS | 39 | -14.772 |
| 5.829 | -0.151 | 1.00 | 0.00 | BED ATOM | 585 | CG MET | 35 | -4.294 | 8.419 | -11.222 | 1.00 | 0.00 | BED ATOM | 679 | HE2 LYS | 39 | -14.772 |
| 4.098 | -0.151 | 1.00 | 0.00 | BED ATOM | 586 | HE1 MET | 35 | -6.361 | 8.419 | -11.222 | 1.00 | 0.00 | BED ATOM | 680 | HE2 LYS | 39 | -14.772 |
| 5.829 | -0.151 | 1.00 | 0.00 | BED ATOM | 587 | HE2 MET | 35 | -6.361 | 8.419 | -11.222 | 1.00 | 0.00 | BED ATOM | 681 | HE1 LYS | 39 | -14.772 |
| 4.098 | -0.151 | 1.00 | 0.00 | BED ATOM | 588 | HN MET | 35 | -6.361 | 8.419 | -11.222 | 1.00 | 0.00 | BED ATOM | 682 | HE2 LYS | 39 | -14.772 |
| 5.829 | -0.151 | 1.00 | 0.00 | BED ATOM | 589 | HN MET | 35 | -6.361 | 8.419 | -11.222 | 1.00 | 0.00 | BED ATOM | 683 | HE1 LYS | 39 | -14.772 |
| 4.098 | -0.151 | 1.00 | 0.00 | BED ATOM | 590 | CA MET | 35 | -5.995 | 8.419 | -11.222 | 1.00 | 0.00 | BED ATOM | 684 | HE2 LYS | 39 | -14.772 |
| 5.829 | -0.151 | 1.00 | 0.00 | BED ATOM | 591 | CA MET | 35 | -5.995 | 8.419 | -11.222 | 1.00 | 0.00 | BED ATOM | 685 | HE1 LYS | 39 | -14.772 |
| 4.098 | -0.151 | 1.00 | 0.00 | BED ATOM | 592 | CA MET | 35 | -5.995 | 8.419 | -11.222 | 1.00 | 0.00 | BED ATOM | 686 | HE2 LYS | 39 | -14.772 |
| 5.829 | -0.151 | 1.00 | 0.00 | BED ATOM | 593 | HE1 MET | 35 | -11.084 | 8.419 | -11.222 | 1.00 | 0.00 | BED ATOM | 687 | HE2 LYS | 39 | -14.772 |
| 4.098 | -0.151 | 1.00 | 0.00 | BED ATOM | 594 | HE2 MET | 35 | -11.084 | 8.419 | -11.222 | 1.00 | 0.00 | BED ATOM | 688 | HE1 LYS | 39 | -14.772 |
| 5.829 | -0.151 | 1.00 | 0.00 | BED ATOM | 595 | HE1 PRO | 35 | -11.084 | 8.419 | -11.222 | 1.00 | 0.00 | BED ATOM | 689 | HE2 LYS | 39 | -14.772 |
| 4.098 | -0.151 | 1.00 | 0.00 | BED ATOM | 596 | HE2 PRO | 35 | -11.084 | 8.419 | -11.222 | 1.00 | 0.00 | BED ATOM | 690 | HE1 LYS | 39 | -14.772 |
| 5.829 | -0.151 | 1.00 | 0.00 | BED ATOM | 597 | HE1 PRO | 35 | -11.084 | 8.419 | -11.222 | 1.00 | 0.00 | BED ATOM | 691 | HE2 LYS | 39 | -14.772 |
| 4.098 | -0.151 | 1.00 | 0.00 | BED ATOM | 598 | HE2 PRO | 35 | -11.084 | 8.419 | -11.222 | 1.00 | 0.00 | BED ATOM | 692 | HE1 LYS | 39 | -14.772 |
| 5.829 | -0.151 | 1.00 | 0.00 | BED ATOM | 599 | HE1 PRO | 35 | -11.084 | 8.419 | -11.222 | 1.00 | 0.00 | BED ATOM | 693 | HE2 LYS | 39 | -14.772 |
| 4.098 | -0.151 | 1.00 | 0.00 | BED ATOM | 600 | HE2 PRO | 35 | -11.084 | 8.419 | -11.222 | 1.00 | 0.00 | BED ATOM | 694 | HE1 LYS | 39 | -14.772 |
| 5.829 | -0.151 | 1.00 | 0.00 | BED ATOM | 601 | HE1 PRO | 35 | -11.084 | 8.419 | -11.222 | 1.00 | 0.00 | BED ATOM | 695 | HE | | |

REPLACEMENT SHEET

REPLACEMENT SHEET

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|-------|---------|------|------|----------|------|----------|----|--------|---|-------|--------|------|------|----------|------|---------|----|--------|-------|--------|------|------|----------|------|-----------|----|--------|
| 6.359 | -9.88 | 1.00 | 0.00 | BED ATOM | 1099 | ME ARG | 66 | 15.162 | - | 3.727 | -2.548 | 1.00 | 0.00 | BED ATOM | 1193 | HEI LVS | 71 | 14.024 | 6.842 | -2.049 | 1.00 | 0.00 | BED ATOM | 1287 | C ALA | 76 | 2.240 |
| 5.351 | -0.277 | 1.00 | 0.00 | BED ATOM | 1100 | HE ARG | 66 | 15.688 | - | 4.084 | -1.699 | 1.00 | 0.00 | BED ATOM | 1194 | HE2 LVS | 71 | 12.561 | 4.601 | -1.147 | 1.00 | 0.00 | BED ATOM | 1288 | O ALA | 76 | 2.240 |
| 5.255 | -11.059 | 1.00 | 0.00 | BED ATOM | 1101 | CQ ARG | 66 | 15.801 | - | 4.316 | -2.655 | 1.00 | 0.00 | BED ATOM | 1195 | N2 LVS | 71 | 14.287 | 4.936 | -3.777 | 1.00 | 0.00 | BED ATOM | 1289 | N ALA | 76 | 2.270 |
| 5.457 | -9.074 | 1.00 | 0.00 | BED ATOM | 1102 | NHL ARG | 66 | 15.917 | - | 3.897 | -3.076 | 1.00 | 0.00 | BED ATOM | 1196 | M2 LVS | 71 | 13.870 | 4.014 | -0.044 | 1.00 | 0.00 | BED ATOM | 1290 | N HL | 77 | 3.124 |
| 5.526 | -7.965 | 1.00 | 0.00 | BED ATOM | 1103 | HILL ARG | 66 | 15.959 | - | 3.334 | -4.556 | 1.00 | 0.00 | BED ATOM | 1197 | HE2 LVS | 71 | 14.334 | 3.685 | -0.394 | 1.00 | 0.00 | BED ATOM | 1291 | CA ALA | 77 | 1.058 |
| 5.372 | -7.7 | 1.00 | 0.00 | BED ATOM | 1104 | HILL ARG | 66 | 14.188 | - | 3.353 | -4.604 | 1.00 | 0.00 | BED ATOM | 1198 | M2 LVS | 71 | 15.253 | 3.804 | -0.818 | 1.00 | 0.00 | BED ATOM | 1292 | HA ALA | 77 | 4.650 |
| 5.314 | -0.071 | 1.00 | 0.00 | BED ATOM | 1105 | NHL ARG | 66 | 17.125 | - | 3.533 | -3.604 | 1.00 | 0.00 | BED ATOM | 1199 | C LVS | 71 | 9.041 | 4.701 | -0.750 | 1.00 | 0.00 | BED ATOM | 1293 | C2 ASP | 77 | 1.392 |
| 5.314 | -0.071 | 1.00 | 0.00 | BED ATOM | 1106 | HILL ARG | 66 | 17.654 | - | 3.160 | -0.231 | 1.00 | 0.00 | BED ATOM | 1200 | O LVS | 71 | 2.156 | 3.524 | -0.283 | 1.00 | 0.00 | BED ATOM | 1294 | HB1 ASP | 77 | 2.156 |
| 5.277 | -9.807 | 1.00 | 0.00 | BED ATOM | 1107 | HE2 ARG | 66 | 17.813 | - | 2.529 | -0.362 | 1.00 | 0.00 | BED ATOM | 1201 | N LVS | 72 | 9.970 | 2.157 | -2.334 | 1.00 | 0.00 | BED ATOM | 1295 | HB2 ASP | 77 | 0.521 |
| 5.075 | -0.692 | 1.00 | 0.00 | BED ATOM | 1108 | O ARG | 66 | 10.634 | - | 4.888 | -0.211 | 1.00 | 0.00 | BED ATOM | 1202 | RH LVS | 72 | 9.933 | 5.201 | -1.059 | 1.00 | 0.00 | BED ATOM | 1296 | CC O2 ASP | 77 | 1.817 |
| 5.075 | -0.692 | 1.00 | 0.00 | BED ATOM | 1109 | N ARG | 66 | 11.634 | - | 4.888 | -0.211 | 1.00 | 0.00 | BED ATOM | 1203 | CA LVS | 72 | 7.844 | 5.201 | -1.059 | 1.00 | 0.00 | BED ATOM | 1297 | CC O2 ASP | 77 | 1.353 |
| 5.759 | -0.613 | 1.00 | 0.00 | BED ATOM | 1110 | HN TTR | 67 | 8.411 | - | 4.618 | -1.255 | 1.00 | 0.00 | BED ATOM | 1204 | LVS | 72 | 7.396 | 4.864 | -1.255 | 1.00 | 0.00 | BED ATOM | 1298 | C LVS | 77 | 2.613 |
| 5.280 | -1.004 | 1.00 | 0.00 | BED ATOM | 1111 | HN TTR | 67 | 8.016 | - | 4.864 | -0.547 | 1.00 | 0.00 | BED ATOM | 1205 | CH LVS | 72 | 8.167 | 5.595 | -2.453 | 1.00 | 0.00 | BED ATOM | 1299 | C ASP | 77 | 0.268 |
| 5.301 | -1.142 | 1.00 | 0.00 | BED ATOM | 1112 | CH TTR | 67 | 6.952 | - | 4.864 | -0.547 | 1.00 | 0.00 | BED ATOM | 1206 | HBL LVS | 72 | 8.161 | 2.641 | -0.243 | 1.00 | 0.00 | BED ATOM | 1300 | O ASP | 77 | -0.950 |
| 5.066 | -9.840 | 1.00 | 0.00 | BED ATOM | 1113 | CB TTR | 67 | 7.982 | - | 7.226 | -0.752 | 1.00 | 0.00 | BED ATOM | 1207 | HB2 LVS | 72 | 7.249 | 7.226 | -0.752 | 1.00 | 0.00 | BED ATOM | 1301 | N LVS | 71 | 2.156 |
| 5.181 | -9.639 | 1.00 | 0.00 | BED ATOM | 1114 | CBP TTR | 67 | 6.767 | - | 6.869 | -2.008 | 1.00 | 0.00 | BED ATOM | 1208 | HB1 LVS | 72 | 9.136 | 1.569 | -0.119 | 1.00 | 0.00 | BED ATOM | 1302 | CB LVS | 78 | 1.944 |
| 5.061 | -11.738 | 1.00 | 0.00 | BED ATOM | 1115 | HB1 TTR | 67 | 6.767 | - | 6.869 | -2.008 | 1.00 | 0.00 | BED ATOM | 1209 | HB2 LVS | 72 | 9.130 | 1.569 | -0.119 | 1.00 | 0.00 | BED ATOM | 1303 | CB LVS | 78 | 0.319 |
| 5.291 | -14.512 | 1.00 | 0.00 | BED ATOM | 1116 | CBP TTR | 67 | 8.216 | - | 6.713 | -7.985 | 1.00 | 0.00 | BED ATOM | 1210 | HB2 LVS | 72 | 9.135 | 1.569 | -0.119 | 1.00 | 0.00 | BED ATOM | 1304 | HA LEBU | 78 | -0.493 |
| 5.541 | -14.516 | 1.00 | 0.00 | BED ATOM | 1117 | CBP TTR | 67 | 7.042 | - | 7.005 | -3.027 | 1.00 | 0.00 | BED ATOM | 1211 | CD LVS | 72 | 8.419 | 6.272 | -0.027 | 1.00 | 0.00 | BED ATOM | 1305 | CH LVS | 78 | -1.280 |
| 5.220 | -13.733 | 1.00 | 0.00 | BED ATOM | 1118 | CBP TTR | 67 | 7.188 | - | 6.184 | -3.147 | 1.00 | 0.00 | BED ATOM | 1212 | CD LVS | 72 | 8.419 | 6.272 | -0.027 | 1.00 | 0.00 | BED ATOM | 1306 | CH LVS | 78 | -1.280 |
| 5.285 | -10.973 | 1.00 | 0.00 | BED ATOM | 1119 | CD TTR | 67 | 8.122 | - | 6.065 | -3.815 | 1.00 | 0.00 | BED ATOM | 1213 | HD2 LVS | 72 | 9.135 | 1.569 | -0.119 | 1.00 | 0.00 | BED ATOM | 1307 | CD LVS | 78 | -1.284 |
| 5.677 | -14.266 | 1.00 | 0.00 | BED ATOM | 1120 | CD TTR | 67 | 8.645 | - | 6.065 | -3.815 | 1.00 | 0.00 | BED ATOM | 1214 | HD2 LVS | 72 | 9.135 | 1.569 | -0.119 | 1.00 | 0.00 | BED ATOM | 1308 | CD LVS | 78 | -1.284 |
| 5.234 | -14.604 | 1.00 | 0.00 | BED ATOM | 1121 | CEL TTR | 67 | 6.767 | - | 6.767 | -6.767 | 1.00 | 0.00 | BED ATOM | 1215 | CEL LVS | 72 | 7.249 | 7.226 | -0.752 | 1.00 | 0.00 | BED ATOM | 1309 | CE LVS | 78 | -0.388 |
| 5.301 | -14.604 | 1.00 | 0.00 | BED ATOM | 1122 | CEL TTR | 67 | 6.261 | - | 6.261 | -6.261 | 1.00 | 0.00 | BED ATOM | 1216 | CEL LVS | 72 | 7.249 | 7.226 | -0.752 | 1.00 | 0.00 | BED ATOM | 1310 | CE LVS | 78 | -0.388 |
| 5.066 | -9.840 | 1.00 | 0.00 | BED ATOM | 1123 | HEI TTR | 67 | 7.982 | - | 6.869 | -2.008 | 1.00 | 0.00 | BED ATOM | 1217 | HEI LVS | 72 | 9.136 | 1.569 | -0.119 | 1.00 | 0.00 | BED ATOM | 1311 | HEI LEBU | 78 | -1.143 |
| 5.734 | -8.684 | 1.00 | 0.00 | BED ATOM | 1124 | HEI TTR | 67 | 7.872 | - | 6.869 | -2.008 | 1.00 | 0.00 | BED ATOM | 1218 | HE2 LVS | 72 | 9.136 | 1.569 | -0.119 | 1.00 | 0.00 | BED ATOM | 1312 | HE2 LEBU | 78 | -0.319 |
| 5.055 | -8.684 | 1.00 | 0.00 | BED ATOM | 1125 | HE2 TTR | 67 | 8.198 | - | 6.869 | -2.008 | 1.00 | 0.00 | BED ATOM | 1219 | HE2 LVS | 72 | 9.136 | 1.569 | -0.119 | 1.00 | 0.00 | BED ATOM | 1313 | HE2 LEBU | 78 | -0.319 |
| 5.490 | -6.639 | 1.00 | 0.00 | BED ATOM | 1126 | HE2 TTR | 67 | 8.216 | - | 6.869 | -2.008 | 1.00 | 0.00 | BED ATOM | 1220 | HE2 LVS | 72 | 9.136 | 1.569 | -0.119 | 1.00 | 0.00 | BED ATOM | 1314 | HE2 LEBU | 78 | -0.319 |
| 5.778 | -7.032 | 1.00 | 0.00 | BED ATOM | 1127 | HE2 TTR | 67 | 8.234 | - | 6.869 | -2.008 | 1.00 | 0.00 | BED ATOM | 1221 | HE2 LVS | 72 | 9.136 | 1.569 | -0.119 | 1.00 | 0.00 | BED ATOM | 1315 | HE2 LEBU | 78 | -0.319 |
| 5.327 | -6.548 | 1.00 | 0.00 | BED ATOM | 1128 | HE2 TTR | 67 | 8.252 | - | 6.869 | -2.008 | 1.00 | 0.00 | BED ATOM | 1222 | HE2 LVS | 72 | 9.136 | 1.569 | -0.119 | 1.00 | 0.00 | BED ATOM | 1316 | HE2 LEBU | 78 | -0.319 |
| 5.027 | -6.548 | 1.00 | 0.00 | BED ATOM | 1129 | HE2 TTR | 67 | 8.270 | - | 6.869 | -2.008 | 1.00 | 0.00 | BED ATOM | 1223 | HE2 LVS | 72 | 9.136 | 1.569 | -0.119 | 1.00 | 0.00 | BED ATOM | 1317 | HE2 LEBU | 78 | -0.319 |
| 5.027 | -6.548 | 1.00 | 0.00 | BED ATOM | 1130 | HE2 TTR | 67 | 8.288 | - | 6.869 | -2.008 | 1.00 | 0.00 | BED ATOM | 1224 | HE2 LVS | 72 | 9.136 | 1.569 | -0.119 | 1.00 | 0.00 | BED ATOM | 1318 | HE2 LEBU | 78 | -0.319 |
| 5.172 | -7.283 | 1.00 | 0.00 | BED ATOM | 1131 | HE2 TTR | 67 | 8.306 | - | 6.869 | -2.008 | 1.00 | 0.00 | BED ATOM | 1225 | HE2 LVS | 72 | 9.136 | 1.569 | -0.119 | 1.00 | 0.00 | BED ATOM | 1319 | HE2 LEBU | 78 | -0.319 |
| 5.051 | -7.283 | 1.00 | 0.00 | BED ATOM | 1132 | HE2 TTR | 67 | 8.324 | - | 6.869 | -2.008 | 1.00 | 0.00 | BED ATOM | 1226 | HE2 LVS | 72 | 9.136 | 1.569 | -0.119 | 1.00 | 0.00 | BED ATOM | 1320 | HE2 LEBU | 78 | -0.319 |
| 5.051 | -7.283 | 1.00 | 0.00 | BED ATOM | 1133 | HE2 TTR | 67 | 8.342 | - | 6.869 | -2.008 | 1.00 | 0.00 | BED ATOM | 1227 | HE2 LVS | 72 | 9.136 | 1.569 | -0.119 | 1.00 | 0.00 | BED ATOM | 1321 | HE2 LEBU | 78 | -0.319 |
| 5.172 | -7.283 | 1.00 | 0.00 | BED ATOM | 1134 | HE2 TTR | 67 | 8.360 | - | 6.869 | -2.008 | 1.00 | 0.00 | BED ATOM | 1228 | HE2 LVS | 72 | 9.136 | 1.569 | -0.119 | 1.00 | 0.00 | BED ATOM | 1322 | HE2 LEBU | 78 | -0.319 |
| 5.051 | -7.283 | 1.00 | 0.00 | BED ATOM | 1135 | HE2 TTR | 67 | 8.378 | - | 6.869 | -2.008 | 1.00 | 0.00 | BED ATOM | 1229 | HE2 LVS | 72 | 9.136 | 1.569 | -0.119 | 1.00 | 0.00 | BED ATOM | 1323 | HE2 LEBU | 78 | -0.319 |
| 5.172 | -7.283 | 1.00 | 0.00 | BED ATOM | 1136 | HE2 TTR | 67 | 8.396 | - | 6.869 | -2.008 | 1.00 | 0.00 | BED ATOM | 1230 | HE2 LVS | 72 | 9.136 | 1.569 | -0.119 | 1.00 | 0.00 | BED ATOM | 1324 | HE2 LEBU | 78 | -0.319 |
| 5.172 | -7.283 | 1.00 | 0.00 | BED ATOM | 1137 | HE2 TTR | 67 | 8.414 | - | 6.869 | -2.008 | 1.00 | 0.00 | BED ATOM | 1231 | HE2 LVS | 72 | 9.136 | 1.569 | -0.119 | 1.00 | 0.00 | BED ATOM | 1325 | HE2 LEBU | 78 | -0.319 |
| 5.172 | -7.283 | 1.00 | 0.00 | BED ATOM | 1138 | HE2 TTR | 67 | 8.432 | - | 6.869 | -2.008 | 1.00 | 0.00 | BED ATOM | 1232 | HE2 LVS | 72 | 9.136 | 1.569 | -0.119 | 1.00 | 0.00 | BED ATOM | 1326 | HE2 LEBU | 78 | -0.319 |
| 5.172 | -7.283 | 1.00 | 0.00 | BED ATOM | 1139 | HE2 TTR | 67 | 8.450 | - | 6.869 | -2.008 | 1.00 | 0.00 | BED ATOM | 1233 | HE2 LVS | 72 | 9.136 | 1.569 | -0.119 | 1.00 | 0.00 | BED ATOM | 1327 | HE2 LEBU | 78 | -0.319 |
| 5.172 | -7.283 | 1.00 | 0.00 | BED ATOM | 1140 | HE2 TTR | 67 | 8.468 | - | 6.869 | -2.008 | 1.00 | 0.00 | BED ATOM | 1234 | HE2 LVS | 72 | 9.136 | 1.569 | -0.119 | 1.00 | 0.00 | BED ATOM | 1328 | HE2 LEBU | 78 | -0.319 |
| 5.172 | -7.283 | 1.00 | 0.00 | BED ATOM | 1141 | HE2 TTR | 67 | 8.486 | - | 6.869 | -2.008 | 1.00 | 0.00 | BED ATOM | 1235 | HE2 LVS | 72 | 9.136 | 1.569 | -0.119 | 1.00 | 0.00 | BED ATOM | 1329 | HE2 LEBU | 78 | -0.319 |
| 5.172 | -7.283 | 1.00 | 0.00 | BED ATOM | 1142 | HE2 TTR | 67 | 8.504 | - | | | | | | | | | | | | | | | | | | |

REPLACEMENT SHEET

REPLACEMENT SHEET

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|--------|--------|------|------|----------|------|------|-----|-----|--------|
| 4.534 | 5.217 | 1.00 | 0.00 | BRC ATOM | 1845 | CN1 | TIR | 115 | 4.662 |
| 0.515 | 6.373 | 1.00 | 0.00 | BRC ATOM | 1846 | HDL1 | TIR | 116 | 3.970 |
| 0.073 | 4.870 | 1.00 | 0.00 | BRC ATOM | 1847 | HDL2 | TIR | 116 | 4.212 |
| 0.238 | 7.147 | 1.00 | 0.00 | BRC ATOM | 1848 | HDL3 | TIR | 116 | 5.046 |
| 0.085 | 6.812 | 1.00 | 0.00 | BRC ATOM | 1849 | HDL4 | TIR | 116 | 5.002 |
| 1.755 | 6.053 | 1.00 | 0.00 | BRC ATOM | 1850 | O | TIR | 116 | 7.024 |
| 0.544 | 6.125 | 1.00 | 0.00 | BRC ATOM | 1851 | N | TIR | 116 | 6.222 |
| 2.465 | 6.014 | 1.00 | 0.00 | BRC ATOM | 1852 | HN | ASP | 117 | 6.079 |
| 1.424 | 8.874 | 1.00 | 0.00 | BRC ATOM | 1853 | CA | ASP | 117 | 5.805 |
| 1.965 | 10.275 | 1.00 | 0.00 | BRC ATOM | 1854 | HA | ASP | 117 | 5.197 |
| 2.585 | 10.798 | 1.00 | 0.00 | BRC ATOM | 1855 | CB | ASP | 117 | 4.967 |
| 0.609 | 10.101 | 1.00 | 0.00 | BRC ATOM | 1856 | HBL | ASP | 117 | 5.564 |
| 0.267 | 10.220 | 1.00 | 0.00 | BRC ATOM | 1857 | HB2 | ASP | 117 | 4.664 |
| 0.596 | 6.976 | 1.00 | 0.00 | BRC ATOM | 1858 | CG | ASP | 117 | 3.722 |
| 0.963 | 10.968 | 1.00 | 0.00 | BRC ATOM | 1859 | OD1 | ASP | 117 | 2.897 |
| 2.220 | 12.889 | 1.00 | 0.00 | BRC ATOM | 1860 | OD2 | ASP | 117 | - |
| 1.624 | 13.480 | 1.00 | 0.00 | BRC ATOM | 1861 | C | ASP | 117 | 3.572 |
| 1.066 | 11.154 | 1.00 | 0.00 | BRC ATOM | 1862 | O | ASP | 117 | 7.006 |
| 0.992 | 12.209 | 1.00 | 0.00 | BRC ATOM | 1863 | N | LVS | 118 | 6.846 |
| 1.897 | 10.725 | 1.00 | 0.00 | BRC ATOM | 1864 | HN | LVS | 118 | 8.206 |
| 2.384 | 9.879 | 1.00 | 0.00 | BRC ATOM | 1865 | CA | LVS | 118 | 8.282 |
| 0.613 | 11.186 | 1.00 | 0.00 | BRC ATOM | 1866 | HA | LVS | 118 | 9.416 |
| 1.946 | 11.488 | 1.00 | 0.00 | BRC ATOM | 1867 | CB | LVS | 118 | 10.248 |
| 2.063 | 10.968 | 1.00 | 0.00 | BRC ATOM | 1868 | HBL | LVS | 118 | 9.315 |
| 1.972 | 12.327 | 1.00 | 0.00 | BRC ATOM | 1869 | HB2 | LVS | 118 | 8.636 |
| 4.975 | 13.133 | 1.00 | 0.00 | BRC ATOM | 1870 | CG | LVS | 118 | 10.292 |
| 2.199 | 13.349 | 1.00 | 0.00 | BRC ATOM | 1871 | HGL | LVS | 118 | 8.918 |
| 3.456 | 12.895 | 1.00 | 0.00 | BRC ATOM | 1872 | HC2 | LVS | 118 | 8.95 |
| 7.119 | 12.286 | 1.00 | 0.00 | BRC ATOM | 1873 | CD | LVS | 118 | 9.857 |
| 3.946 | 13.191 | 1.00 | 0.00 | BRC ATOM | 1874 | HOJ | LVS | 118 | 10.477 |
| 4.608 | 12.327 | 1.00 | 0.00 | BRC ATOM | 1875 | HO2 | LVS | 118 | 10.468 |
| 5.794 | 11.631 | 1.00 | 0.00 | BRC ATOM | 1876 | CE | LVS | 118 | 9.208 |
| 5.425 | 10.502 | 1.00 | 0.00 | BRC ATOM | 1877 | HE1 | LVS | 118 | 8.302 |
| 6.386 | 12.369 | 1.00 | 0.00 | BRC ATOM | 1878 | HE2 | LVS | 118 | 8.697 |
| 6.652 | 10.963 | 1.00 | 0.00 | BRC ATOM | 1879 | NZ | LVS | 118 | 10.212 |
| 6.458 | 11.316 | 1.00 | 0.00 | BRC ATOM | 1880 | HE1 | LVS | 118 | 11.463 |
| 7.656 | 11.096 | 1.00 | 0.00 | BRC ATOM | 1881 | HE2 | LVS | 118 | 9.989 |
| 6.459 | 9.921 | 1.00 | 0.00 | BRC ATOM | 1882 | HE3 | LVS | 118 | 10.206 |
| 11.10 | 11.551 | 1.00 | 0.00 | BRC ATOM | 1883 | C | LVS | 118 | 9.557 |
| 10.802 | 10.802 | 1.00 | 0.00 | BRC ATOM | 1884 | OCT1 | LVS | 118 | 9.047 |
| 0.641 | 10.802 | 1.00 | 0.00 | BRC ATOM | 1885 | OCT2 | LVS | 118 | 10.454 |
| 0.302 | 12.459 | 1.00 | 0.00 | BRC END | | | | | |